Chapter 3
Methodology

3-1.0 Goals and definitions

As discussed in Chapter 1, the goal of this method is to extrapolate from available pesticide toxicity data for a limited number of species to a concentration that should not produce detrimental physiological effects in aquatic life. These criteria aim to protect all species in the ecosystem. This goal is derived from narrative toxicity objectives listed in the Basin Plan (CVRWQCB 2004). This methodology was designed for the Sacramento and San Joaquin River watersheds, but is generally applicable to freshwater ecosystems in the United States. Simple modifications could be made to adapt this method for saltwater criteria or other geographic areas.

3-1.1 Relevant compounds

This method is intended for deriving water quality criteria for pesticides. The term pesticide is defined by the Central Valley Regional Water Quality Control Board (CVRWQCB 2004) as (1) any substance or mixture of substances that is intended to be used for defoliating plants, regulating plant growth, or for preventing, destroying, repelling, or mitigating any pest, which may infest or be detrimental to vegetation, man, animals, or households, or be present in any agricultural or nonagricultural environment whatsoever, or (2) any spray adjuvant, or (3) any breakdown products of these materials that threaten beneficial uses. Sources of pesticide inputs into the Sacramento River and San Joaquin River basins include runoff and drainage from agriculture, silviculture, and residential and industrial storm water (CVRWQCB 2004). Certain procedures were derived using only data on organic pesticides and may not be appropriate for metals or other compounds. This is noted in the assessment factor section (3-3.3) and in the default ACR section (3-4.2.3).

3-1.2 Notes about numeric criteria

As discussed in the Phase I report (TenBrook & Tjeerdema 2006, TenBrook *et al.* 2009) water quality criteria are referred to by different terms and are used for different purposes depending upon how they are derived. For this project, numeric criteria are science-based values, which are intended to protect aquatic life from adverse effects of pesticides, without consideration of defined water body uses, societal values, economics, or other nonscientific considerations. Criteria and guidelines are not formally established, nor are they themselves water quality objectives. Criteria derived using this method do not represent CVRWQCB policy and are not regulations. Also, while this method uses data from the pesticide registration process, the method is not intended to replace the risk assessment work performed by the pesticide regulatory agencies.

3-1.3 Overview

This methodology consists of a combination of features from existing methodologies with refinements based on recent research in aquatic ecotoxicology and environmental risk assessment. Components were selected based on evaluations and recommendations in the Phase I report (TenBrook & Tjeerdema 2006, TenBrook *et al.* 2009) and in Chapter 2 of this Phase II report. This methodology includes components for deriving water quality criteria from both large and small data sets. For a given compound, the criteria derivation method will depend on the richness of the available data. Figures 3.1 and 3.2 are flow-charts summarizing procedures for collection, evaluation, and reduction of data sets, and for acute and chronic criteria derivation. Due to the large number of figures and tables in this chapter, all are presented at the end of the report to improve readability of the text. The methodology is presented in the format of a standard operating procedure.

3-2.0 Data

This section provides details of how to collect, summarize, evaluate and reduce data to be used in criteria derivation.

3-2.1 Collect data

Utilizing the sources listed in Table 3.1, collect physical-chemical and ecotoxicity data for the pesticide of concern. This is not an exhaustive list, but does contain sufficient resources to find virtually all available physical-chemical and ecotoxicity data for a given pesticide. Table 3.2 gives web addresses for electronic resources. Table 3.3 lists the kinds of physical-chemical and ecotoxicity data that should be collected.

Physical Chemical data should be collected first as it aids in the interpretation of toxicity data studies (see section 3-2.2.2). The other data in Table 3.3 is used for considerations after criteria are derived or for other aspects of data interpretation. Much of the physical-chemical data can be collected relatively quickly from the handbooks listed in Table 3.1 and this section does not need to be an extensive review. For K_{ow} values, the LOGKOW database is recommended (Sangster Research Laboratories 2004).

Ecotoxicity data should include studies of aquatic organisms exposed to a pesticide via water. Do not collect terrestrial toxicity data (see section 3-2.1.2.3 for exception), including laboratory rat and mice studies, and studies with in vitro exposures of organs or tissues (i.e., were not whole-body exposures). As this methodology is for derivation of criteria in the United States, only data for freshwater species that are members of families with reproducing populations in North America will be used for criteria derivation, but all data should be collected as it may be used for supporting information or for derivation of an acute-to-chronic ratio (ACR). EPA guidelines have an appendix that lists species resident in North America (EPA 1985). Literature searches should go back far enough to cover from the time a pesticide was first developed to the present.

Any and all original study reports should be sought out from agencies, peer reviewed literature and other sources. Unpublished study reports can be collected from EPA by reviewing a RED (Reregistration Eligibility Decisions) report and requesting appropriate studies through the freedom of information act. Local state pesticide regulation agencies may have copies of such unpublished reports as well. See Table 3.1 for details. Data from agencies can make up most of the high quality toxicity studies available, especially for compounds with limited data. Information from agencies should be requested first since it can be very useful and can take several weeks to receive information.

The rest of this section provides specific guidance and definitions regarding what kinds of ecotoxicity data should be collected.

3-2.1.1 Single-species laboratory aquatic toxicity data

Single-species laboratory aquatic toxicity data are the type of data that will be used directly for criteria calculation. They are derived from laboratory tests with aquatic species using aqueous exposures (do not collect data from sediment, topical, or oral exposures). Field and multi-species data (including systems with both water and soil/sediment) will be considered later. These data may be acute or chronic, have several endpoints, and be expressed in different terms as described below.

3-2.1.1.1 Definitions of acute and chronic toxicity data

Acute:

1) Crustacean or insect tests with exposures lasting 24-96 h; (RIVM 2001; Siepmann & Finlayson 2000; USEPA 1985; 2003b);
2) Fish, mollusk or amphibian tests with exposures lasting 96 h (RIVM 2001);
3) Shellfish embryo, larval, or older life-stage tests with exposures lasting 96 h (USEPA 1985; 2003b).

Plant/algae toxicity tests usually measure endpoints generally associated with chronic toxicity, such as growth and reproduction. Therefore, explicit definitions for acute plant/algae tests are not included.

Chronic (all from USEPA 1985; 2003d):

1) Plant/algae, single-celled organism tests of any exposure duration;
2) Any test that takes into account the number of young produced, regardless of exposure duration;
3) Full life-cycle exposure tests (ranging from 7 d for mysids to 15 months for salmonids);
4) Partial life-cycle exposure tests (all major life stages exposed in less than 15 mo; specifically for fish that require more than a year to reach sexual maturity);

5) Early life-stage exposure tests (ranging from 28-60 d; also specifically for fish).

3-2.1.1.2 Toxicity values

For derivation of acute criteria, obtain LC_{50} or EC_{50} values from acute toxicity tests. For derivation of chronic criteria or acute-to-chronic ratios, obtain maximum acceptable toxicant concentrations (MATCs). Chronic data expressed as EC_x values (from regression analysis), may be used for criteria derivation only if studies are available to show what level of *x* is appropriate to represent a no-effect level.

If not reported in a study, LC_{50} or EC_{50} values may be calculated if raw data are available. Likewise, MATC values can be calculated as the geometric mean of the no observed effect concentration (NOEC) and the lowest observed effect concentration (LOEC). If NOEC or LOEC values are not stated in a report, but data were evaluated statistically, then the following calculations may be made (based on RIVM 2001):

a) The highest reported concentration not statistically different from the control ($p < 0.05$) is the NOEC; the NOEC is needed for calculation of the MATC;

b) The lowest reported concentration that is statistically different from the control ($p < 0.05$) is the LOEC; the LOEC is needed for calculation of the MATC;

c) For a MATC expressed as a range of values, the NOEC is the lower value, the LOEC is the higher value and the MATC may be calculated as the geometric mean, as described previously.

3-2.1.1.3 Toxicity endpoints

Appropriate endpoints for criteria derivation are those that measure survival, growth, or reproductive effects. This includes measures of immobility, as well as population level endpoints, such as r (intrinsic rate of population growth) and λ (factor by which a population increases in a given time). Endpoints other than survival, immobility, growth, reproduction, r, or λ may be used in criteria derivation if those endpoints have been linked to effects on survival, growth, or reproduction. For example, if a study has determined that an 80% effect on acetylcholinesterase (AChE) inhibition is significant (in either an acute or chronic exposure), and if 80% AChE inhibition is shown to lead to mortality *for that species*, then an IC_{80} value (concentration that causes 80% inhibition compared to the control) may be used as a toxicity value in criteria derivation. Alternatively, if that same study determined a lowest observed effect concentration (LOEC) that represents 80% reduction from control, then the corresponding maximum acceptable toxicant concentration (MATC) value from that study may be used in criteria derivation or for derivation of an acute-to-chronic ratio. It is important to emphasize that levels of sub-lethal effects that lead to reductions in survival, growth, or reproduction are species specific. If no data are available linking effects such as endocrine disruption, enzyme induction, enzyme inhibition, behavioral effects, histological effects, stress protein induction, changes in RNA or DNA levels, mutagenicity, and carcinogenicity to

survival, growth or reproduction, these data are not to be used directly for criteria derivation.

3-2.1.2 Other ecotoxicity data

Single-species laboratory aquatic toxicity data (described in the previous section 3-2.1.1) will be used directly for criteria derivation. Other data described in the next three subsections may be used to check or modify criteria, depending on availability, in sections 3-5.0 to 3-7.0.

3-2.1.2.1 Multispecies (field/semi-field/laboratory) data

Multi-species data are not used directly for criteria derivation. However, they should be collected because multispecies laboratory, field, or semi-field data are used in section 3-6.2 for comparison to criteria derived from single-species data (OECD 1995; RIVM 2001), and may provide justification for adjustment of a final criterion (RIVM 2001; USEPA 1985; 2003b; Zabel & Cole 1999).

3-2.1.2.2 Water quality effects data

After criteria are derived with single-species studies, other information will be considered in the water quality effects section including: the effects of suspended particulate matter on bioavailability, the effects of pesticide mixtures, and the effects of temperature, pH, or other water quality parameters on toxicity. These data should be collected as well. It is recommended that these specific sections be reviewed first to know what kind of studies will be useful.

3-2.1.2.3 Terrestrial and human health data

Although these criteria are not intended for protection of human or terrestrial life, a separate section is included to address bioaccumulation or secondary poisoning in terrestrial organisms that may be indirectly exposed from feeding on aqueous species that have pesticide in their tissues. This section is only required if the compound is likely to bioaccumulate, therefore, this section should be reviewed before collecting the required wildlife and human health data (section 3-7.1).

3-2.2 Evaluate data

In this section, instruction is given for how to determine if data are relevant and reliable for use in deriving water quality criteria.

3-2.2.1 Physical-chemical data

Evaluate physical-chemical data according to whether it was obtained by an appropriate method that was properly used. Table 3.4 indicates acceptable methods for determination of a number of physical-chemical parameters other than K_{ow}. Table 3.5

indicates acceptable methods specifically for determination of K_{ow} values. The methods shown in Table 3.5 are listed in order of preference; computational methods should only be used if no measured data are available. The recommended values in the LOGKOW database (Sangster Research Laboratories 2004) may be used without further review because they have been thoroughly reviewed before inclusion in the database. Physical-chemical parameters reported by manufacturers may also be used without further review as they are widely accepted, and original studies are usually not published. Physical-chemical parameters determined by methods not shown in Tables 3.4 and 3.5 (or equivalent methods) should be used with caution.

3-2.2.2 Ecotoxicity data

Use the physical-chemical data to evaluate ecotoxicity studies. Water solubility is needed to compare to tested concentrations to check that none of the compound precipitated. Half-life ($t_{1/2}$), partition coefficients (K_{OC}, K_{OW}, K_H), and vapor pressure are important to determine if a compound will dissipate rapidly in a static test, making a flow-though exposure more appropriate. Tests that report toxicity values greater than 2x the geometric mean of available water solubility values for the pesticide are not useful even as supporting information and can be eliminated without further consideration. For compounds with log K_{OW} between 5 and 7, laboratory tests should use feeding regimes that minimize or eliminate interaction of pesticide with food particles.

Ecotoxicity data will be evaluated for relevance and reliability. For the single-species tests, evaluate the relevance using the rating system in Table 3.6 and assign a rating of R (relevant), L (less relevant) or N (not relevant) based on the scale in Table 3.11. Tests that score < 70 (i.e., rating = N) do not need to be evaluated further, but it is useful to create a brief record of the citation and list of the relevance parameters not fulfilled. All single-species tests with a relevance score $\geq$ 70 (i.e., rating = R or L) should be summarized. A data sheet, like Figure 3.4, helps to ensure that all relevant information is drawn from each study. In the data sheets, report all toxicity values from different time points, endpoints or repeated tests. The most appropriate values will be selected later in the data reduction procedures. Using the data in these sheets, and the rating systems shown in Tables 3.7 and 3.8, evaluate single-species aquatic ecotoxicity studies on two aspects of reliability: 1) documentation; and 2) acceptability.

Evaluate other types of aquatic toxicity tests (i.e., multispecies laboratory/field, microcosm, mesocosm) on documentation and acceptability using Table 3.9. Evaluate terrestrial toxicity studies based solely on documentation using Table 3.10. Assign reliability ratings to each study of R (reliable), L (less reliable) or N (not reliable) based on the scale in Table 3.11. Specific instructions for rating various kinds of ecotoxicity studies are given below.

<u>Single-species laboratory studies (aquatic species with aqueous exposures)</u>

1) Rate relevance using the scoring system in Table 3.6; if, and only if, the relevance score is ≥ 70, go on to the following steps; if the relevance score is < 70, the test is not usable and does not need to be evaluated further;
2) Fill in data summary (Fig 3.4);
3) Rate documentation using the scoring system in Table 3.7;
4) Rate acceptability using the scoring system in Table 3.8;
5) Average the scores from 2 and 3 for an overall reliability rating;
6) Assign the study to a category based on reliability and relevance scores according to Table 3.11;
7) Use studies rated RR for criteria derivation; use studies rated RL, LR or LL as supporting data; do not use studies receiving N ratings.

Aquatic outdoor field data/indoor model ecosystems (including microcosms/mesocosms), multi-species data

1) Rate documentation and acceptability using the scoring system in Table 3.9.
2) Assign a reliability rating of R, L, or N using the scoring system in Table 3.11.
3) Use studies rated R or L to evaluate potential ecosystem effects (section 3-6.2); do not use studies rated N.

Terrestrial wildlife data

1) Rate documentation using scoring system in Table 3.10.
2) Assign a reliability rating of R, L, or N using the scoring system in Table 3.11.
3) Use studies rated R or L to assess potential hazards due to pesticide bioaccumulation (section 3-7.1); do not use studies rated N.

Organize single-species data into tables with at least the genus, species, value(s), and reference. Create different tables for acute data rated RR, chronic data rated RR, the supplemental data (rated RL, LL, LR), and data excluded from calculations as part of the reduction process. If a study has results from multiple tests with the same species report each value as an individual test by the same author. These toxicity values will be combined when data is reduced.

3-2.3 Fill chronic toxicity data gaps with estimation techniques

Chronic data sets may be supplemented with extrapolation techniques that estimate chronic toxicity based on acute toxicity data called time-concentration-effect (TCE) analysis. These data may be used in species sensitivity distribution (SSD) criteria derivation procedures (section 3-3.2), but not in an acute-to-chronic ratio (section 3-4.2). Specific taxa requirements are needed to do the chronic toxicity SSD. Values from TCE may be used to fulfill these taxa requirements to perform the SSD. To estimate chronic toxicity values, the ACE program requires acute mortality data with three components: exposure concentration, degree of response, and time course of effect. This requires having access to raw toxicity data that includes exposure concentrations and measurements of mortality at multiple time points.

If there are appropriate acute data that could be used to estimate chronic data for use in the SSD, perform time-concentration-effect (TCE) analysis using USEPA's acute-to-chronic estimation software (ACE, v. 2.0, Ellersieck *et al.* 2003, available for free download at http://www.epa.gov/ceampubl/fchain/index.htm). The software comes with a user's manual that fully explains the models used, explains how to choose a model, describes model limitations, and gives guidance on how to use the software. The ACE program output provides estimated toxicity values for a range of mortality levels and a range of chronic exposure periods. For the accelerated life testing (ALS) model, a 1% mortality level is recommended to represent a NOEC, while for the multifactor probit analysis (MPA) and linear regression analysis (LRA) models a 0.01% effect level is recommended (Ellersieck *et al.* 2003). The exposure period should be selected to reflect a full life-cycle of the organism used in the acute study. Full documentation of the ACE program is included in Appendix 3A.

3-2.4 Reduce data

For criteria derivation, data must be reduced such that each species has one representative data point in the final data set. In cases where there is more than one toxicity value for a species, reduce data to a single species mean acute value (SMAV) or species mean chronic value (SMCV).

Following are the specific data reduction procedures:

1) Calculate SMAVs/SMCVs as the geometric mean of toxicity values from one or more acceptable tests with the same endpoints (ANZECC & ARMCANZ 2000; ECB 2003; OECD 1995; RIVM 2001; USEPA 1985; 2003b);

2) If data are available for life stages that are at least a factor of two more resistant than another life stage for the same species, then use the data for the more sensitive life stage to calculate the SMAV because the goal is to protect all life stages (RIVM 2001; USEPA 1985; 2003b);

3) If data are available for one species, but for multiple appropriate endpoints (see section 3-2.1.1.3), then use the data for the most sensitive endpoint (ANZECC & ARMCANZ 2000; ECB 2003; OECD 1995; RIVM 2001);

4) If a NOEC is not explicitly reported in chronic toxicity studies, but statistical analysis was done, the NOEC may be determined as the highest reported concentration not statistically different from the control ($p < 0.05$, RIVM 2001); the NOEC is not used in criteria derivation, but is needed for calculation of the MATC;

5) Similarly, if a LOEC is not explicitly reported in chronic toxicity studies, it may be determined as the lowest reported concentration that is statistically different from the control ($p < 0.05$); the LOEC is not used in criteria derivation, but is needed for calculation of the MATC;

6) If a MATC is not reported, it may be calculated as the geometric mean of the NOEC and LOEC;

7) If no toxicity values were reported, but raw data are available, calculate toxicity values using appropriate statistical methods (ECB 2003);

8) If a MATC is expressed as a range of values, recalculate the MATC as the geometric mean of the high and low values (RIVM 2001);

9) If reasons for differences between tests for the same species/endpoints are found, then data may be grouped according to appropriate factors (e.g., pH or temperature; ECB 2003). Selection of the appropriate value to use in criteria derivation should be based on standard test parameters. Tests conducted under non-standard conditions (vs. standard conditions as defined in standard test methods) may be used to derive quantitative relationships between those conditions and toxicity (as in USEPA 1985; 2003b). If such a relationship is established then toxicity values derived under non-standard conditions may be translated to standard conditions and added to the criteria derivation data set. If no quantitative relationship can be derived then tests conducted under non-standard conditions should not be used for criteria derivation, but may be used as supporting information.

10) If data are available for multiple time points from crustacean or insect acute toxicity studies use the latest time point (i.e., 96-h tests are preferred over tests of < 96 h);

11) For a given species, use data from flow-through tests in which concentrations were measured, if it is available. If such data are not available, then data from static or static-renewal tests and/or tests in which concentrations were not measured may be used as long as they are rated otherwise relevant and reliable.

3-2.5 Graph data

Construct a histogram of the frequency distribution (see Chapter 2 section 2-3.1.1 for examples). Examine the distribution for multimodality (see section 3-3.2.5, part a) or outliers. Double-check toxicity values for errors, especially toxicity values that appear to be outliers. A multi-modal distribution may be more easily seen when graphing a cumulative frequency distribution. This can be done as part of the SSD fitting in the next sections or a graph of cumulative frequency vs. log concentration can be constructed using equation 3.1 below. If a distribution is used to calculate a final criterion, a graph of the distribution plotted with the actual toxicity values should be included in the final report.

$$\text{Cumulative frequency} = \frac{rank - 0.5}{n} \qquad (3.1)$$

where:

rank = position in set of ordered data (ranked from lowest to highest)
n = sample number

Once data are collected, evaluated, selected, and reduced, criteria derivation may begin.

3-3.0 Derive acute criterion

If five acute data requirements can be fulfilled (see below) a species sensitivity distribution (SSD) will be used to derive the acute criterion in section 3-3.2. Otherwise an AF will be used in section 3-3.3.

3-3.1 Data requirements for the species sensitivity distribution (SSD)

Collect, evaluate, and reduce data as described in sections 3-2.0 through 3-2.4. For derivation of acute or chronic criteria by the SSD method a minimum of five data from five different families are required. For the chronic value for an herbicide use the procedure in section 3-4.3, but an acute criterion should be derived if possible with animal data. The data set must include:

a) The family Salmonidae;
b) A warm water fish;
c) A planktonic crustacean, of which one must be in the family Daphniidae in the genus *Ceriodaphnia, Daphnia,* or *Simocephalus*;
d) A benthic crustacean;
e) An insect (aquatic exposure).

If these five requirements are met, then use the SSD method described in section 3-3.2 to derive the acute criterion. If such data are not available, then use the AF method described in section 3-3.3.

3-3.2 Derive criterion using a SSD

Depending on the number of species mean toxicity values, the Burr III distribution (3-3.2.1) or the log-logistic distribution (3-3.2.2) will be used. Combine data from all taxa for this procedure, but data on plants and algae should be kept separate. From the fitted distribution, determine the concentrations that will protect 95% of species with 50% confidence (95:50), 95% of species with 95% confidence (95:95), 99% of species with 50% confidence (99:50), and 99% of species with 95% confidence (99:95). The number that is most robust of these is the one selected to protect 95% of species with 50% confidence. This median 5^{th} percentile estimate is recommended for derivation of the acute criterion. The other numbers may be used if more conservative numbers are desired, but since they come from the extreme tails of the SSD they are less reliable.

3-3.2.1 Burr III SSD, for 8 or more toxicity values

Derive criteria using the SSD method described in ANZECC & ARMCANZ (2000). Using any statistical package that is capable, fit the data to a Burr Type III distribution (Burr III, inverse Weibull, or inverse Pareto; Burr 1942), and calculate the 1st and 5th percentile values using the following equations (record to three significant figures):

$$PC(q) = \frac{b}{\left[\left(\frac{1}{1-q}\right)^{\frac{1}{k}} - 1\right]^{\frac{1}{c}}} \qquad (3.2)$$

where:

$PC(q)$ is the protecting concentration that will protect q% of species; thus, the 5th percentile is calculated by setting q = 95;
q = percent of species to protect;
b, c, k are fit parameters.

For reciprocal Weibull (for cases when $k \to \infty$):

$$PC(q) = (-\alpha / \ln(1-q))^{1/b} \qquad (3.3)$$

where:

$PC(q)$ and q are as described for Burr III;
α and β are fit parameters.

For reciprocal Pareto (for cases when $c \to \infty$):

$$PC(q) = x_0 (1-q)^{1/\theta} \qquad (3.4)$$

where:

$PC(q)$ and q are as described for Burr III;
x_0 and θ are fit parameters.

Note that it is acceptable to use any statistical package that can fit Burr Type III distributions to accomplish this calculation and the calculation of confidence limits discussed in the following section. The BurrliOZ program, which was developed specifically for use in deriving target values (criteria) in the ANZECC & ARMCANZ (2000) methodology, is available for free from the CSIRO website at http://www.cmis.csiro.au/Envir/burrlioz/. Documentation and information for this program are included in Appendix 3A. The BurrliOZ software comes with a caution that

for data sets of eight or fewer toxicity values, there will be great uncertainty in the calculated values. The software authors provide a procedure to follow in such cases. This procedure has been modified for this method and is presented in section 3-3.2.2.

Perform the fit test as in section 3-3.2.4 and calculate confidence limits 3-3.2.3.

3-3.2.2 Log-logistic SSD, for 8 or fewer toxicity values

When there are 8 or fewer toxicity values in the data set preference should be given to using the log-logistic distribution over the Burr III distribution. Note: the BurrliOZ software comes with a specific procedure to compare the fit of log-logistic distribution to the Burr Type III distribution and use the one that appears to fit better (see readme file, included in Appendix 3A). This is a modification of that procedure and is to be used in place of that procedure.

Fit the data to a log-logistic distribution using a statistics package capable of the analysis. An example of such a program, ETX v.1.3 (Aldenberg 1993) is documented in Appendix 3A and software can be obtained from RIVM by contacting info@rivm.nl. Once the fit parameters (α and β) have been determined, utilize the following equation to determine 1st and 5th percentile values:

$$p = \frac{100}{1 + \exp(-[\ln(x) - \alpha]/\beta)} \qquad (3.5)$$

where:

p = percentage of species unaffected at x; set p = 1 to calculate the 1st percentile; p = 5 for the 5th percentile
x = toxicity value at p;
α = sample mean (of ln(x));
$\beta = k_L \cdot s_n/C_5$.

and:

k_L = extrapolation constant; dependent on sample size; selected for either median or lower 95th percentile estimate (see Table 3.12);
s_n= sample standard deviation (of ln(x)); n = sample size;
C_5 = constant = 2.9444.

Note: some software uses log(x) in place of ln(x) in equation 3.5 and to calculate α and β, such as the ETX v. 1.3 software. If using α and β calculated from log(x), be sure also to use log(x) in the equation 3.5 instead of ln(x).

Perform the fit test as in section 3-3.2.4.

If the fit of the data to the log-logistic distribution passed the fit test ($p > 0.05$)

then this distribution should be used to calculate the 1st and 5th percentile values for the data set. If the log-logistic distribution fails the fit test, then use the procedure in section 3-3.2.1 to fit the Burr Type III distribution.

3-3.2.3 Calculate confidence limits

The values calculated in section 3-3.2.1 represent median estimates of the 1st and 5th percentiles. To estimate the lower 95% confidence limit for these estimates, utilize the following bootstrapping technique (CSIRO 2001):

1) Resample the original data set, with replacement, to create a new data set the same size as the original set and calculate 1st and 5th percentile values from the new data set. Repeat this resampling and recalculation procedure 200-1000 times. At least 501 resamplings are recommended (ANZECC & ARMCANZ 2000); fewer will give a less certain estimate; more will give a more certain estimate, but will require more calculation time.

2) Order the bootstrapped estimates from lowest to highest (separately for the 1st and 5th percentile SSD estimates) and select the 5th percentile value; this represents the lower 95% confidence limit estimate of the 1st or 5th percentile of the SSD.

These procedures can be accomplished using the program BurrliOZ v. 1.0.13 (CSIRO 2001). Full documentation is available in Appendix 3A. The software can be obtained at http://www.cmis.csiro.au/Envir/burrlioz/. Also the ETX v.1.3 software (Aldenberg 1993) calculates the 95% confidence limit for the 5th percentile estimate for the log-logistic distribution, but not for 1st percentile. The latter estimate may be omitted for log-logistic distribution since the other three are likely to be more useful because they have less uncertainty.

3-3.2.4 Check the goodness of fit of the SSD

The following procedure checks that the SSD fits the toxicity data. The BurrliOZ software chooses the best fitting SSD with a goodness of fit based on maximum likelihood estimation, this is a different approach based on cross-validation. In general, this approach starts by omitting the first data point and refitting the distribution. Then the probability of the omitted point is estimated with the new distribution. This is done for each data point in turn and the combined results for all points in the data set is examined for a significant lack of fit using Fisher's combined test, outlined below.

The distribution will have been fitted based on a sample of n species toxicity values, which are concentrations and can also be called x values (as in plotting y vs. x). Refit this distribution based on the data set that *omits* the point x_i. This distribution function is called F_{-i}. Then assess the placement of the omitted point within this distribution, called $F_{-i}(x_i)$. Solving for $F_{-i}(x_i)$ calculates the corresponding probability for x_i (which would also be called the y value). In the BurrliOZ software, after you refit the distribution, the results window allows entry of a concentration (x_i) and then provides the corresponding percentile, solving for $F_{-i}(x_i)$. Determine $F_{-i}(x_i)$ for each data point.

Then let

$$p_i = 2 * min\ (F_{-i}(x_i), 1 - F_{-i}(x_i)),$$

where '*min*' indicates using the minimum of either $F_{-i}(x_i)$ or $1 - F_{-i}(x_i)$.

Apply Fisher's combined test and calculate a chi squared statistic of the form

$$X^2_{2n} \sim -2 \sum_i ln(p_i)$$

If any one of the data points is fitted poorly enough then the test is capable of rejecting the hypothesis that the data come from the fitted (BurrIII) distribution. Once all of the p_i values have been calculated, the chi squared statistic (X^2) is calculated. (In Excel the significance of chi squared statistic is calculated with the command:

CHIDIST, with the fields (x, deg freedom),

where x = $-2 \sum_i ln(p_i)$

and deg freedom is the degrees of freedom or n, the number of p_i values.)

The closer the resulting value for X^2_{2n} is to 1, the better the fit. When the result for $X^2_{2n} <$ 0.05 there is a significant effect from the substitution and a 95% probability of a significant lack of fit. The data should then be critically examined and checked for multi-modality, and a different procedure may be used as described in section 3-2.5 and Figure 3.3.

3-3.2.5 Procedure if SSD does not fit

If the full data set cannot be fit to a SSD (procedure described in sections 3-3.2.1 and 3-3.2.2) examine the data for multi-modality and/or outliers as outlined in the steps below. If appropriate, reanalyze using the appropriate procedure for the remaining number of data points and the fulfilled taxa requirements (see Figure 3.3).

a) Examine data for multi-modality. If a SSD cannot be fit and visual inspection indicates that the SSD is multi-modal and this occurs in a justifiable manner (such as by taxa), divide the data into subsets and use the subset containing the lowest toxicity values (ANZECC and ARMCANZ 2000). This is easily done in conjunction with the data plotting step, 3-2.5. A distribution can be fitted to a subset that does not contain the five taxa requirements provided that the original data set fulfilled these requirements and the final subset contains at least five data points.

b) Double-check the toxicity values to be sure they are not mistakes (i.e., typographical or transcriptional errors) and review the original studies again to be sure that all test conditions were appropriate. The need to remove outliers is considerably reduced using the Burr Type III distribution with the BurrliOZ software (CSIRO Biometrics, Campbell

et al. 2000). If a fit cannot be obtained with a larger data set, critical examination of data is emphasized as any one point outlier that causes the SSD to not fit likely represents an extreme difference that is erroneous (i.e., above the water solubility of the compound or below the analytical detection limit). If errors are found remove the erroneous data from the data set and use the remaining data. Removal of data from the SSD could also be justified if there is supporting information as to why the outlier(s) does not belong in the same SSD as the remaining data (similar to separating based on multi-modality, e.g., a resistant strain of mosquitoes). This approach is reasonable because, as with all criteria derived from this methodology, criteria will be evaluated to determine if they will provide adequate protection (section 3-6.0).

c) If removal of data is not justifiable and it is not possible to fit a SSD, the assessment factor should be defaulted to. This should be done especially in the cases of 5-8 data as the data is most likely multi-modal but there is not enough data to fit the lower subset. However, keep in mind, with eight points or fewer the procedure instructs to attempt to fit with log-logistic distribution before using the Burr III distribution (see section 3-3.2.2).

3-3.2.6 Calculate criterion from 5th percentile value

For the acute criterion:
The recommended criterion = (5th percentile value at 50% confidence level) ÷ 2

For the chronic criterion:
The recommended criterion = 5th percentile value at the 50% confidence level

Alternatively, more conservative criteria may be derived from other percentile or confidence levels.

The number of significant digits in the final criterion should be consistent with known variability in the calculated criteria. Calculated criteria should not be expressed with more significant figures compared to the original toxicity data. If using the median estimate as the criteria, the 95% confidence limit can be used as a guide. The digit in the median estimate that is different from the 95% confidence limit would indicate the last significant digit. Also, the 5th percentile values generated from omitting data sets during the fit test (section 3-3.2.4) can be used to estimate the uncertainty in the calculated criteria. The last digit that is relatively variable among these estimates indicates the last significant digit.

If toxicity is quantitatively related to a water quality parameter, follow procedures in section 3-5.3 for appropriate expression of the criterion. Criteria will be checked against the individual toxicity values in the data sets used in the SSD in section 3-6.1, to ensure protection of all represented species.

3-3.3 Derive acute criterion using an Assessment factor (AF)

If data requirements for the SSD procedure cannot be met or an SSD cannot be fit, then the AF method must be used to derive criteria. Divide the lowest species mean acute value from the data set by a factor (Table 3.13). The magnitude of the factor is dependent on the number of data requirements met, and at least one of the available, acceptable data must be from the family Daphniidae in the genus *Daphnia*, *Ceriodaphnia*, or *Simocephalus,* or a criterion cannot be calculated. Each of the additional data must be from each of the different families as per the list of those required for the SSD method, such that each additional value is building toward completion of the minimum SSD data set. The resulting value represents an estimate of the median 5th percentile value of the SSD.

Acute criterion = (lowest value in data set ÷ assessment factor) ÷ 2
= estimated 5th percentile value ÷ 2

If toxicity is quantitatively related to a water quality parameter, follow procedures in section 3-5.3 for appropriate expression of the criterion.

It should be noted that these assessment factors were formulated with data from organic insecticides. Some molluscicides, miticides, fungicides have similar properties as well and these factors would serves as a reasonable means of estimating criteria in these cases. These factors should not be used with metal-based pesticides. For herbicides (or if plants are most sensitive), however, another procedure should be used as described in section 3-4.3. The AFs in Table 3.13 may be updated and recalculated as more criteria are generated. Data sets that meet the five taxa requirements for SSD may be added to those originally used in Chapter 2 section 2-3.2 to calculate new AFs.

3-4.0 Derive chronic criterion

If five chronic data requirements can be fulfilled an SSD will be used to derive the chronic criterion (described below), otherwise an ACR will be used (section 3-4.2).

3-4.1 Chronic criterion using an SSD

If at least five chronic toxicity data are available for species from five different families, as described in section 3-3.1 (either from direct measurements or from TCE estimates as described in section 3-2.3), then follow the instructions in section 3-3.2 to determine a chronic 5th and 1st percentile values at various confidence levels. If such data are not available, then proceed to section 3-4.2 for derivation of a chronic criterion by application of an ACR to the acute criterion. For the chronic value for an herbicide, use the procedure in 3-4.3. A chronic value derived by the SSD method does not require any further adjustment by a safety factor because this value is derived from long-term no-effect toxicity values and may be used directly as a criterion.

3-4.2 Chronic criterion using an acute-to-chronic ratio (ACR)

When chronic data are lacking, use acute-to-chronic ratios (ACRs) to extrapolate from acute to chronic toxicity. Preferably ACRs from measured (experimental) toxicity data will be used if they can be calculated. ACRs are derived by following the procedures in sections 3-4.2.1 through 3-4.2.3, in order (taken from ANZECC & ARMCANZ 2000; USEPA 1985; 2003b). If sufficient data is not available to calculate ACRs from measured toxicity data, a default value is provided in section 3-4.2.3. Resulting criteria will be checked against the individual toxicity values in the chronic toxicity data set in section 3-6.1 to ensure protection of all represented species.

3-4.2.1 Single-chemical, multispecies ACR based on measured data

This procedure requires acute and chronic data from organisms in at least three different families including a fish, an invertebrate, and at least one other acutely sensitive species. For each acceptable chronic value (MATC) having at least one corresponding appropriate acceptable acute value, an ACR is calculated by dividing flow-through acute test by the chronic value. Static tests are acceptable for midges, daphnids and other zooplankton. For fish, the acute test(s) should be conducted with juvenile or younger fish. For all species, the acute test(s) should be part of the same study and use the same dilution water as the chronic test. If there are multiple acute tests that are equally appropriate, use the geometric mean of the toxicity values. If acute tests were not conducted as part of the same study, but were conducted as part of a different study in the same laboratory and dilution water, then they may be used. If no such acute tests are available, results of acute tests conducted in the same dilution water in a different laboratory may be used. If there are not enough freshwater data to fulfill the ACR data requirements, then saltwater species may be used because freshwater and saltwater ACRs have been shown to be comparable (USEPA 1985) and this approach has been accepted in numerous criteria derivations (Siepmann & Finlayson 2000; USEPA 1980a; b; c; d; 2003a; 2005).

The species mean acute-to-chronic ratio (SMACR) is calculated for each species as the geometric mean of all ACRs available for that species. For some materials, the ACR seems to be the same for all species, but for other materials the ratio seems to increase or decrease as the SMAV increases. Thus the final, multi-species ACR can be obtained in one of three ways, depending on the data available:

1) If the SMACR seems to increase or decrease as the SMAVs increase, calculate the ACR as the geometric mean of the ACRs for species whose SMAVs are close to the acute criterion (this includes species whose SMACRs are within a factor of 10 of the SMACR of the species whose SMAV is nearest the 5^{th} percentile value);

2) If no major trend is apparent and the ACRs for all species are within a factor of ten, calculate the ACR as the geometric mean of all of the SMACRs;

3) If the most appropriate SMACRs are less than 2.0, and especially if they are less than

1.0, acclimation has probably occurred during the chronic test. In this situation, assume the final ACR to be 2.0, so that the chronic criterion is equal to the acute criterion.

If the data requirements of this section cannot be met, or if the ACR cannot be obtained by one of methods 1, 2 or 3 above, then derive the ACR by the procedure in section 3-4.2.2.

3-4.2.2. Single-chemical, multispecies ACR based on measured toxicity data and/or default ACR values

If not enough data are available for calculation of an ACR according to the procedure in section 3-4.2.1, then derive the ACR by calculating the geometric mean of any available ACRs based on measured data, plus enough default ACRs of 12.4 (described in the next section) to give a total of three ACRs (USEPA 2003b). For example, if no measured ACRs are available, then three assumed, or default, ACRs are used. If two ACRs from measured toxicity data are available, then just one default value is used.

3-4.2.3 Default ACR

The default ACR for pesticides for this methodology is 12.4. Derivation of this value is described in Chapter 2. The only appropriate ACRs found that could be included were from organic insecticides. Some molluscicides, miticides, and fungicides have similar properties as well and these factors would serve as a reasonable means of estimating criteria in these cases. The default ACR should not be used with metals (for possible alternatives see the discussion on the derivation of the default ACR in Chapter 2 and Host *et al.*1995). For herbicides (or if plants are most sensitive), however, another procedure should be used in section 3-4.3. This default ACR may be revised if: 1) data sets collected according to this methodology lead to different ACR values; 2) if previously calculated ACRs are shown to be invalid based on data sets collected according the this methodology; or 3) additional pesticide ACR values become available in other EPA criteria documents (or similar thoroughly vetted criteria documents). In any of these events, the default ACR should be recalculated as the 80^{th} percentile value of the new set of ACRs. Table 3.14 shows the current set of ACRs used to calculate the default value. Any future revisions of the value should start with this data set.

3-4.2.4 Calculation of the chronic criterion

Calculate the chronic criterion by dividing the acute 5^{th} (or 1^{st}) percentile value (derived by the SSD method or estimated by the AF method) by the ACR (derived by one of the three methods in sections 3-4.2.1 through 3-4.2.3). This approach is equivalent to that in the USEPA methodologies which divide the Final Acute Value (i.e., the 5^{th} percentile value) by the ACR to derive the chronic criterion (USEPA 1985; 2003b):

Chronic Criterion = (Selected percentile value) ÷ ACR

If toxicity is quantitatively related to a water quality parameter, follow procedures in section 3-5.3 for appropriate expression of the criterion.

3-4.3 Chronic criterion for an herbicide

For herbicides, alga, or vascular aquatic plant data must be included. Since life cycles of plants vary widely and procedures for conducting toxicity tests with plants are not well developed, explicit definitions for acute plant tests are not included. Therefore, plant data can only be used to derive the chronic criterion and the methodology for herbicides will be as follows.

If the chemical is an herbicide and plants are the most sensitive group:

1) Fit a SSD with only alga or vascular aquatic plant data, if there are data from at least five different species that were rated RR;

2) If there is not enough data to do the SSD as described above, then use the lowest NOEC value from an important alga or vascular aquatic plant species that has measured concentrations and the endpoint is biologically relevant.

Few criteria have been derived for herbicides and in general approaches are not as well described as criteria calculation procedures for other pesticides. This is an area where new approaches are currently being developed. The Minnesota Pollution Control Agency (Angela Preimesberger) is working on criteria development of herbicides. Mark Hanson of University of Manitoba is working on guidance for interpreting plant/algal toxicity data. They and other agencies may be good resources to consult with about how to best work with individual plant data sets.

3-5.0 Incorporate water quality into criteria compliance

If the toxicity of a chemical can be quantitatively related to one or more water quality characteristics then either express criteria in the form of equations that quantify the relationship, or use the relationship to determine site-specific compliance with criteria. For organic pesticides, the water quality characteristics of primary concern are effects of suspended particulate matter on bioavailability, the effects of pesticide mixtures, and the effects of temperature, pH, or other parameters on toxicity. Section 3-5.1 addresses bioavailability; section 3-5.2 presents methods for compliance determination in cases where pesticide mixtures are present; and section 3-5.3 presents methods also used by USEPA (1985; USEPA 2003b) for expression of criteria in the form of equations relating pH, temperature, or other parameters to toxicity.

3-5.1 Bioavailability

If significant levels of suspended and/or dissolved solids co-occur with pesticides in a water body, then it may be desirable to consider the effects of solids on the bioavailability of pesticides in determining compliance with derived criteria. The following approach is recommended:

1) In the water column, pesticides may be sorbed to solids, sorbed to dissolved solids, or freely dissolved in the water. If studies show that all three phases are bioavailable, then compliance must be based on total concentration of pesticide in water. Likewise, if no data are available regarding bioavailable phases for a given pesticide, then compliance must be based on total concentration.

2) If studies establish that fewer than three phases are bioavailable, then compliance may be based on concentrations in the bioavailable phases. The most direct way to determine compliance in this case is to measure concentrations in each phase and determine the total bioavailable concentration. Alternatively, concentration in the dissolved phase may be estimated from measurement of total concentration by using the following three-phase equilibrium partitioning model (Chin & Gschwend 1992):

$$C_{dissolved} = \frac{C_{total}}{1 + ((K_{OC} \cdot [SS]) / f_{oc}) + (K_{DOC} \cdot [DOC])} \qquad (3.6)$$

where: $C_{dissolved}$ = concentration of chemical in dissolved phase (μg/L);
C_{total} = total concentration of chemical in water (μg/L);
K_{OC} = organic carbon-water partition coefficient (L/kg);
$[SS]$ = concentration of suspended solids in water (kg/L);
f_{oc} = fraction of organic carbon in suspended sediment in water;
$[DOC]$ = concentration of dissolved organic carbon in water (kg/L);
K_{DOC} = organic carbon-water partition coefficient (L/kg) for DOC.

The use of this model requires measuring total pesticide concentration in water, as well as total and suspended solids. Site-specific K_{OC} and K_{DOC} values must also be available.

3) To estimate bioavailable concentrations of pesticide without specific knowledge of which phases are bioavailable, passive sampling devices may be of use. However, they have a number of technical limitations and will not be useful for determination of compliance with acute criteria.

3-5.2 Mixtures

As recommended in Phase I (TenBrook & Tjeerdema 2006, TenBrook *et al.* 2009) only the additive concentration addition model (for pesticides with similar modes of action, Plackett & Hewlett 1952) and the non-additive interaction model (for chemicals that display antagonistic or synergistic interactions, Finney 1942) are included in this methodology. Two approaches to using the concentration addition model are

presented. The non-additive interaction model is presented with the caveat that it can only be applied in cases where a valid coefficient of interaction (K) is available (either a multispecies K value, or individual species K values). Without multispecies K values, this technique should not be used to assess compliance with water quality criteria, but K values for individual species could be used to assess the potential harm from non-additive toxicity on a species by species basis. A final caveat is that application of all of these mixture models requires that each pesticide that is considered in the model has a numeric water quality criterion.

3-5.2.1 Concentration addition—for pesticides with similar modes of action

Two equally valid approaches to compliance determination for mixtures of similarly-acting pesticides are presented: the toxic unit approach and the relative potency factor approach (as suggested by Felsot 2005). Regulators may choose which to use.

3-5.2.1.1 Toxic unit approach

According to the toxic unit approach (CVRWQCB 2004), compliance with water quality criteria is determined as follows:

$$\sum_{i=1}^{n} \frac{C_i}{O_i} < 1.0 \qquad (3.7)$$

where:

C_i = concentration of toxicant i in water
O_i = water quality objective/criterion for toxicant i

As long as the sum is < 1.0, the water body is considered to be in compliance with respect to the mixture.

3-5.2.1.2 Relative potency factor (RPF) approach

The relative potency factor (RPF) approach, suggested by Felsot (2005), is analogous to the toxic equivalency factor (TEF) approach used in assessing toxicity of dioxin and dioxin-like compounds (Van Den Berg *et al.* 1998). To use this method for a group of similarly-acting chemicals, select one chemical (usually the most toxic) to be the reference chemical. For each chemical in the group, determine an RPF using the following equation:

$$RPF_i = \frac{Criterion_{xR}}{Criterion_{xi}} \qquad (3.8)$$

where:

RPF_i = relative potency factor

$Criterion_{xR}$ = water quality criterion (acute or chronic) of reference chemical (μg/L)
$Criterion_{xi}$ = water quality criterion (acute or chronic) of the *i*th chemical (μg/L)

Use each RPF value to calculate the toxic equivalents of each component of the mixture with respect to the reference chemical:

$$TE_i = RPF_i * C_i \quad (3.9)$$

where:

TE_i = toxic equivalents of *i*th component of the mixture (μg/L)
RPF_i = relative potency factor of the *i*th component of the mixture
C_i = concentration of the *i*th component of the mixture (μg/L)

Determine compliance with the criterion for the reference chemical using the following equation:

$$TE_{total} = C_R + \sum_{n}^{i} TE_i \quad (3.10)$$

where:

TE_{total} = total toxic equivalents of mixture (μg/L)
C_R = Concentration of reference chemical (μg/L)

If $TE_{total} \leq$ the criterion for the reference compound, then the water body is in compliance.

3-5.2.2 Non-additivity; synergism and antagonism

If a valid, multispecies interaction coefficient (K; discussed in Chapter 2) is available for a known synergist or antagonist over a range of concentrations, then this procedure may be followed to determine compliance of mixtures.

First, determine the adjusted, or effective, concentration of a chemical in the presence of an antagonist or synergist:

$$C_a = C_m(K) \quad (3.11)$$

where:

C_a = adjusted, or effective, concentration of chemical
C_m = concentration measured
K = coefficient of interaction, specific to the synergist/antagonist at a particular concentration

Compare the adjusted concentration to the criterion to determine compliance. Additionally, the adjusted concentration can be used in the additivity models described in section 3-5.2.1. If single-species K values are available over a range of concentrations, this approach may be used to assess potential for harm, but should not generally be used to determine compliance with criteria. However, if the available single-species K values are for one of the most sensitive species in a data set, then this approach may be used to assess compliance.

For mixtures containing both synergists and antagonists, or multiple synergists/antagonists, equation 3.11 can be modified to include multiple K values (LeBlanc, pers. comm. 2006):

$$C_a = C_m(K_1K_2...K_n) \qquad (3.12)$$

where:

C_a and C_m are as defined in equation 3.11
K_1, K_2, K_n = K values for synergist/antagonist 1, 2…n

This multiple-K value approach should not be used to assess compliance, but may be used to assess research needs.

3-5.3 Temperature, pH and other effects (USEPA 1985; 2003b)

Use this procedure (taken directly from USEPA 1985; 2003b) for both acute and chronic data. When enough acceptable data (i.e., rated RR by this methodology) are available to show that toxicity to two or more species (at least one fish and one invertebrate) is similarly related to a water quality characteristic, account for the relationship using analysis of covariance (ANCOVA). The ANCOVA may be done with a computer program, or by the manual procedure outlined below. If two or more factors affect toxicity, use multiple regression analysis. Note that if a quantitative relationship is found at this step, then toxicity values obtained in otherwise acceptable studies conducted under non-standard conditions may be translated to toxicity values at standard conditions and added to the data set. Criteria would then have to be recalculated with the additional data.

3-5.3.1 Regress toxicity values vs. water quality values by species (based on USEPA 1985; 2003b)

For each species for which comparable acute toxicity values from acceptable studies (rated RR) are available at three or more different values of the water quality characteristic, perform a least squares regression of the acute toxicity values on the corresponding values of the water quality characteristic to obtain the slope and its 95% confidence limits for each species. Transform data as necessary to optimize model fits.

3-5.3.2 Assess relevance and reasonableness of data and regressions (based on USEPA 1985; 2003b)

Decide whether the data for each species are relevant, taking into account the range and number of the tested values of the water quality characteristic and the degree of agreement within and between species. For example, a slope based on six data points might be of limited value if it is based only on data for a very narrow range of values of the water quality characteristic. A slope based on only three data points, however, might be useful if it is consistent with other information and if the three points cover a broad enough range of the water quality characteristic. If useful slopes are not available for at least one fish and one invertebrate, or if the available slopes are statistically dissimilar, or if too few data are available to adequately define the relationship between acute toxicity and the water quality characteristic, then criteria should not be expressed as an equation and only results of tests conducted under standard conditions should be used for criteria derivation. If a relationship is established, then results of toxicity tests conducted under non-standard conditions can be translated to standard conditions and added to the criteria derivation data set.

3-5.3.3 Normalize toxicity and water quality values and re-do regression

For each species, calculate the geometric mean of the available acute or chronic toxicity values and then divide each of the toxicity values for the species by the geometric mean for the species. This normalizes the toxicity values so that the geometric mean of the normalized toxicity values for each species individually and for any combination of species is 1.0. Similarly normalize the values of the water quality characteristic for each species individually using the same procedure as above. Individually for each species perform a least squares regression of the normalized acute values of the water quality characteristic on the normalized toxicity values. The resulting slopes and 95% confidence limits will be identical to those obtained above with the non-normalized data, but when the data are plotted the line of best fit for each individual species will go through the point 1,1 in the center of the graph.

3-5.3.4 Combine species to obtain a pooled slope

Treat all of the normalized data as if they were all for the same species and perform a least squares regression of all of the normalized acute values on the corresponding normalized values of the water quality characteristic to obtain the pooled acute slope, V, and its 95% confidence limits. The line of best fit for the standardized data set will go through the point 1,1 in the center of the graph.

3-5.3.5 Calculate toxicity values at Z for each species

For each species calculate the geometric mean, W, of the non-normalized toxicity values and the geometric mean, X, of the values of the non-normalized water quality characteristic.

For each species, calculate Y, the mean toxicity value at a selected value, Z, of the water quality characteristic using the equation:

$$Y = W - V(X - Z) \quad (3.13)$$

where:

V = pooled slope of the regression curve
W = geometric mean of toxicity values for a species (at all levels of the water quality characteristic)
X = geometric mean of water quality characteristics for a species
Y = toxicity value for a species at selected value
Z = selected value of water quality characteristic

If data were transformed prior to derivation of regression slopes, then equation 3.13 will be:

$$\ln Y = \ln W - V(\ln X - \ln Z) \quad (3.14)$$

and the toxicity value is calculated as:

$$e^{Y} \quad (3.15)$$

NOTE: Alternatively, the toxicity values at Z can be obtained by using equation 3.13 or equations 3.14 and 3.15 to adjust each value individually to Z (as opposed to adjusting the geometric mean values), and then calculating the mean of the adjusted values for each species. This alternative procedure allows an examination of the range of the adjusted acute toxicity values for each species.

Derive criteria at Z (i.e., a standard toxicity tests value) by using the toxicity values derived from this procedure and the procedures described in sections 3-3.0 and 3-4.0.

The acute criterion is expressed as:

$$\frac{e^{(V[\ln(\text{waterqualitycharacteristic})]+\ln A - V[\ln Z])}}{2} \quad (3.16)$$

and the chronic criterion is expressed as:

$$e^{(V[\ln(\text{waterqualitycharacteristic})]+\ln A - V[\ln Z])} \quad (3.17)$$

where:

V = pooled acute slope
A = acute or chronic criterion at Z derived from SSD, AF, or ACR procedures

Z = selected value of water quality characteristic

Because V, A, and Z are known, criteria can be calculated for any selected value of the water quality characteristic.

3-6.0 Check criteria against ecotoxicity data

Once derived according to methods discussed in the procedures in section 3-3.0 and 3-4.0, criteria must be evaluated to ensure that they are set at levels that will protect against adverse effects to: 1) particularly sensitive species, 2) ecosystems, and 3) threatened and endangered species (TES). If evidence suggests that the 5^{th} percentile will not be protective, criteria may be adjusted downward. The recommended means of making such an adjustment is to use either a lower 95% confidence limit estimate of the 5^{th} percentile (see discussion in Chapter 2 section 2-3.1.3), or a median or 95% confidence limit estimate of the 1^{st} percentile.

3-6.1 Sensitive species

Derived criteria should be compared to studies of the most sensitive species to ensure that these species will be protected. If a calculated criterion is higher than toxicity values reported for a particularly sensitive species, then the criterion may require downward adjustment. This evaluation should be based only on measured toxicity values from acceptable studies (i.e., those rated RR, RL, LR, or LL).

3-6.2 Ecosystem and other studies

Evaluate the criteria against laboratory, field or semi-field data from acceptable multispecies studies (rated R or L) to judge whether they will be protective of ecosystems. Make this judgment based on reported ecosystem NOEC values, or on NOEC, EC, IC or LC values for individual species within the system. If toxicity values obtained for appropriate endpoints (i.e., those related to survival, growth, or reproduction) in these studies are lower than the derived criteria, then criteria may need to be adjusted downward. Adjustment of criteria upward is not recommended, as single species data have indicated this concentration to be protective and increasing the criteria may cause toxicity to sensitive species.

3-6.3 Threatened and endangered species

Criteria derived to protect the most sensitive species in ecosystems should be protective of threatened and endangered species (TES). However, a few tools are available to investigate this more rigorously. The guidance presented here may be used to assess whether criteria derived by the new methodology will be protective of TES.

First, obtain the latest list of California TES available from the California Department of Fish and Game web site (www.dfg.ca.gov/hcpb/species/t_e_spp/tespp.shtml, CDFG 2006a; b).

Then, for comparison to acute criteria:

1) Compare criteria to toxicity values from acceptable studies of effects on TES.

2) If no toxicity values are available for a TES, but an acceptable acute toxicity value is available for a surrogate species in the same family or genus as the TES, then use the ICE program (v. 1.0; available at http://www.epa.gov/ceampubl/fchain/index.htm) to estimate a toxicity value for the TES (Asfaw *et al.* 2003, documentation provided in Appendix 3A). Compare this estimated value to the acute criterion.

3) If no surrogate value is available, and if the chemical of interest has a narcotic mode of action, select a QSAR (e.g., from OECD 1995; RIVM 2001) that can be used to estimate toxicity to the TES or to a surrogate based on a log K_{ow} value. Note that while many industrial chemicals have a narcotic mode of action, very few pesticides fall into this category. Fumigants (e.g., methyl bromide, naphthalene, chloropicrin, and others) are a class of pesticides with a narcotic mode of action (USEPA 2006).

For comparison to chronic criteria:

1) Compare criteria to toxicity values from acceptable studies of effects on TES.

2) If no surrogate value is available, and if the chemical of interest has a narcotic mode of action, select a QSAR (e.g., from OECD 1995; RIVM 2001) that can be used to estimate toxicity to the TES or to a surrogate based on a log K_{ow} value.

The QSARs from RIVM (2001) and OECD (1995) are given in Table 3.16. These are presented as examples and do not preclude the use of other QSARs that may be established in published studies in the future.

If no data for the TES or acceptable surrogates are available, and if no applicable QSARs are available, then no special methods are available to assess whether the criteria will be protective of these species, but protection of TES is expected since criteria are derived based on protecting all species. If any of the above comparisons reveal that a criterion is higher than any of the TES toxicity values (or estimated toxicity values), then the criterion may need to be adjusted downward.

3-7.0 Consider partitioning to other environmental compartments

These criteria should also be checked if they might be conflict with any existing guidelines for 1) wildlife and human health due to bioaccumulation and 2) other environmental compartments due to partitioning of chemicals from the water compartment. Information that indicates the criteria may be in conflict with other protection goals should be flagged for further review by environmental managers. Results of these sections should not be used to alter final criteria.

3-7.1 Bioaccumulation/secondary poisoning

For bioaccumulative chemicals it is important to be sure that water quality criteria are set at levels that do not lead to unacceptable levels of chemicals in food items. This section presents a procedure for checking calculated chronic criteria for the possibility of secondary poisoning of wildlife, or possible human health effects, due to bioaccumulation in fish or other food items. Acute criteria do not require this check because they are intended to protect against short periods of elevated pesticide concentrations, making the equilibrium model inappropriate. For wildlife, this requires the availability of studies that demonstrate adverse effects from dietary intake of toxicants; for human health, this requires the availability of FDA action limits for the chemical of concern.

First, determine if the chemical of interest is known to bioaccumulate, or has the potential to bioaccumulate. This includes chemicals that have been shown to bioaccumulate in well-conducted studies (i.e., consistent with standard methods), or have one or more of the following characteristics: $\log K_{ow} > 3$, (ECB 2003; OECD 1995); molecular weight < 1000, (OECD 1995); molecular diameter < 5.5 Å (OECD 1995); molecular length < 5.5 nm (OECD 1995); solid-water partition coefficient ($\log K_d$) > 3; highly adsorbent (ECB 2003), or; belong to a class of chemicals that are known to be bioaccumulative (ECB 2003). Chemicals are not expected to bioaccumulate if they are reactive and/or readily metabolized.

The next steps only apply if a chemical is bioaccumulative, or has the potential to bioaccumulate, and if dietary toxicity data or FDA action levels are available. For effects on humans obtain FDA action level for fish tissues. For effects on wildlife, obtain toxicity values from wildlife with significant food sources in water. Often Mallard duck toxicity values are generated for pesticide registration and available from EPA (see Table 3.1). A chronic NOEC is the best toxicity value to use in this section, but sub-acute toxicity values may be used if a NOEC is not available. Three common oral wildlife toxicity values are described below:

1) Acute (LC_{50}): one time dose, usually force fed (oral gavage/ intubation), and the toxicity value is reported as mg/kg body weight. Since this value is expressed per body weight and not a feed concentration it is not recommended for use in this section.
2) Sub-acute (LC_{50}): in which the compound is in the feed and fed to the animals for 2 weeks to months, and the toxicity value is usually reported as ppm feed.
3) Chronic (NOEC & LOEC): similar exposure to a sub-acute study, but reproduction is monitored.

Also measured (preferred) or estimated BCF, BMF and/or BAF values for food items are required for the calculation. Use the following equation to translate dietary NOEC or LC_{50} values, or FDA action levels, into water NOEC values (adapted from ECB 2003):

$$NOEC_{water} = \frac{NOEC_{oral-predator}}{BCF_{food\_item} \cdot BMF_{food\_item}} \quad (3.18)$$

or:

$$NOEC_{water} = \frac{LC_{50,oral-predator}}{BCF_{food\_item} \cdot BMF_{food\_item}} \quad (3.19)$$

where:

$NOEC_{water}$ = NOEC in water; concentration in water below this level is not expected to lead to bioaccumulation to harmful levels in food items;
$NOEC_{oral\_predator}$ = dietary NOEC value for wildlife or FDA action level (mg pesticide/kg food);
$LC_{50,oral\_predator}$ = dietary LC_{50} value for wildlife (mg pesticide/kg food);
BCF_{food_item} = bioconcentration factor; ratio of concentration of chemical in tissue of food item due to water-only exposure to concentration in water; whole-body, wet-weight value (ECB 2003; OECD 1995; USEPA 1985; 2003b);
BMF_{food_item} = biomagnification factor in food item; ratio of concentration of chemical in predator to concentration in prey items; lipid-normalized, if possible (ECB 2003).

If no measured BCF is available, a value can be estimated using the log K_{ow} from the following linear free energy relationship (Mackay 1982), which was derived for chemicals with log K_{ow} values ranging from ~2 to ~7:

$$\log BCF = \log K_{ow} - 1.32 \quad (3.20)$$

Crosby (1998) cautions that predictions using this equation are less accurate for compounds with log BCF values above 5 or below 2. If equation 3.20 gives a result outside this range, then a more appropriate LFER should be sought in the literature.

If no measured BMF is available, use an appropriate default value from Table 3.15 (based on log K_{ow} or BCF, ECB 2003). Note that the default BMF values based on log K_{OW} in Table 3.15 represent high estimates in light of studies showing no biomagnification of compounds with log K_{OW} values < 6 (Berglund *et al.* 2000; Varó *et al.* 2002). In the case of chlorpyrifos (log K_{ow} = 4.96), Varó *et al.* (2002) attribute the lack of biomagnification, in part, to the biotransformation and depuration ability of organisms at higher trophic levels. For compounds that are readily biotransformed, the default values based on BCF should be used in favor of those based on log K_{OW}.

Alternatively, if a bioaccumulation factor (BAF) is available for fish, then equation 3.18 is modified to:

$$NOEC_{water} = \frac{NOEC_{oral-predator}}{BAF_{fish}} \quad (3.21)$$

where:

$NOEC_{water}$ = NOEC in water;
$NOEC_{oral\_predator}$ = dietary NOEC for wildlife or FDA action level (mg pesticide/kg food);
BAF_{fish} = bioaccumulation factor in fish; ratio of concentration of chemical in tissue due to water plus dietary exposure to concentration in water; lipid-normalized for chemicals with log $K_{ow} > 3$.

Equation 3.19 can be modified in the same way, substituting BAF for (BCF*BMF).

If no BAF value is available, then equation 3.18 or 3.19 must be used, and if no measured BMF value is available, then the appropriate default value should be used (Table 3.15). If multiple BCF, BAF or BMF values are available for a chemical, the geometric mean of all acceptable values should be used.

To determine compliance, compare the $NOEC_{water}$ derived from one of the equations in this section to the water quality criterion. If it is above the criterion, then no adjustment of the criterion is necessary. If the $NOEC_{water}$ is below the criterion, then indicate in the final criteria statement that these criteria may not be protective of all beneficial uses based on the bioaccumulation/secondary poisoning section and that additional review is needed. Discussion of such additional review is beyond the scope of this methodology.

3-7.2 Harmonization with air or sediment criteria

Pesticides in the water may sorb to sediment or volatilize into the air and cause toxicity to organisms in those compartments. Steady-state environmental models may be used to assess harmony, or coherence, of chronic criteria across all environmental media. As this analysis is based on equilibrium partitioning, it is not necessary to consider acute criteria. If there are no levels of concern established for sediment, air, or biota compartments, then there is no need to use this procedure. Concern for bioaccumulation/secondary poisoning that may affect wildlife or human health is addressed by the procedure outlined in section 3-7.1. Acceptable, freely available models include:

1) Exposure Analysis Modeling System (EXAMS, Burns 2004) available from the USEPA Center for Exposure Assessment Modeling (CEAM; http://www.epa.gov/ceampubl/swater/index.htm). The user manual is included in Appendix 3A; the software can be downloaded directly from the USEPA website.

2) MacKay's Fugacity-Based Environmental Equilibrium Partitioning Models (Mackay 2001), from the Canadian Environmental Monitoring Center (CEMC;

http://www.trentu.ca/cemc/). The user manuals for Levels I, II and III are included in Appendix 3A; the software can be downloaded directly form the CEMC website.

The different fate models vary in complexity, and require the use of default environmental parameter values when measured values are not available, but they can provide rough estimates of equilibrium concentrations of chemicals in all environmental compartments based on a given concentration in water (i.e., the chronic criterion concentration) and a few physical-chemical parameters for the chemical.

Because of its relative ease of use, the Level I fugacity model is recommended as a rough first-pass evaluation of equilibrium concentrations. In using this model, the total mass of chemical in the system is adjusted until the equilibrium concentration in water is at the chronic criterion level. The model should be run over a range of values for parameters that may affect equilibria (e.g., organic carbon levels or fish lipid levels). If no harmonization problems are apparent from a series of Level I analyses (i.e., steady-state concentrations in all compartments are below their respective levels of concern), then no further analysis is necessary. However, if any problems are identified, then site-specific data should be obtained to allow more refined modeling.

For all models used, state all input parameters, conditions and assumptions. Compare model outputs, based on having a chemical of concern at its chronic criterion level in water, to appropriate levels of concern established for the non-water compartments (e.g., sediment or air quality criteria or FDA action levels). If the steady-state concentrations in all compartments are acceptable then the water quality criterion is acceptable. If the concentration in a non-water compartment is projected to exceed a concentration of concern, then indicate so in the final criteria statement that these criteria may not be protective of all beneficial uses based on the harmonization/coherence across media section and that additional review is needed. Discussion of such additional review is beyond the scope of this methodology.

3-8.0 Review assumptions and limitations to derived criteria

The assumptions, limitations, and uncertainties involved in criteria generation should be available to inform environmental managers of the accuracy and confidence in criteria. Chapter 2 discusses these points for each section as different procedures were chosen, such as the list of assumptions associated with using an SSD, included in section 2-3.1.5.1, and reviews them in section 2-7.0. This section should summarize any data limitations that affected the procedure used to determine the final criteria. The final criteria statement (in section 3-9.0) should also briefly review these points making it obvious how the final criterion was derived. An example of an important limitation affecting the derivation process would be missing taxa requirement that required use of assessment factors. The different calculations of distributional estimates included in section 3-3.2.1 may be used to consider the uncertainty in the resulting criteria. These different estimates may also be suggested for use as criteria if other considerations (section 3-6.0) show the standard median estimate is likely to be under protective. The considerations in section 3-5.0 and 3-6.0 may indicate other important data limitations

that should be included here. Finally, criteria reports should be periodically reviewed and the most recent literature incorporated.

3-9.0 State final criteria

Very briefly summarize procedures used to calculate criteria and include reference to corresponding sections, if this was not done in the previous section. Final criteria statements should briefly review any other considerations (from section 3-6) that may be important for policy makers to consider.

Criteria will be stated as follows (based on USEPA 1985; 2003b):

Aquatic life should not be affected unacceptably if the four-day average concentration of (1) does not exceed (2) μg/L more than once every three years on the average and if the one-hour average concentration does not exceed (3) μg/L more than once every three years on average.

where:

(1) = insert name of chemical
(2) = insert the chronic criterion
(3) = insert the acute criterion

These averaging periods and the frequency of exceedance may be modified if data and/or models become available that can scientifically defend altering them.

3-10.0 References

Aldenberg T. 1993. ETX 1.3a. A program to calculate confidence limits for hazardous concentrations based on small samples of toxicity data. National Institute of Public Health and the Environment (RIVM), Bilthoven, The Netherlands.

Aldenberg T, Slob W. 1993. Confidence limits for hazardous concentrations based on logistically distributed NOEC toxicity data. *Ecotoxicol Environ Saf* 25:48-63.

ANZECC, ARMCANZ. 2000. Australian and New Zealand guidelines for fresh and marine water quality. Australian and New Zealand Environment and Conservation Council and Agriculture and Resource Management Council of Australia and New Zealand, Canberra, Australia.

Asfaw, A., M.R. Ellersieck, and F.L. Mayer. 2003. Interspecies correlation estimations (ICE) for acute toxicity to aquatic organisms and wildlife. II. User manual and software. U.S. Environmental Protection Agency Report No. EPA/600/R-03/106, Washington, DC. 20 p. + software.

ASTM. 1997. Standard test method for partition coefficient (n-octanol/water) estimation by liquid chromatography. E 1147-92. *Annual Book of Standards*. West Conshohocken, PA: American Society for Testing and Materials.

Berglund O, Larsson P, Ewald G, Okla L. 2000. Bioaccumulation and differential partitioning of polychlorinated biphenyls in freshwater, planktonic food webs. *Can J Fish Aquat Sci* 57:1160-1168.

Burns LA. 2004. Exposure analysis modeling system (EXAMS): User manual and system documentation, Revision G. US Environmental Protection Agency, Washington, DC.

Burr IW. 1942. Cumulative frequency functions. *Annals of Mathematical Statistics* 13:215-232.

Calamari D, Galassi S, Setti F, Vighi M. 1983. Toxicity of selected chlorobenzenes to aquatic organisms. *Chemosphere* 12:253-262.

Call DJ, Brooke LT, Knuth ML, Poirier SH, Hoglund MD. 1985. Fish subchronic toxicity prediction model for industrial organic chemicals that produce narcosis. *Environ Toxicol Chem* 4:335-341.

CCME. 1999. A protocol for the derivation of water quality guidelines for the protection of aquatic life. Canadian Environmental Quality Guidelines. Canadian Council of Ministers of the Environment, Ottawa.

CDFG. 2006a. State and federally listed endangered, threatened animals of California. California Natural Diversity Database available at www.dfg.ca.gov/hcpb/species/t_e_spp/tespp.shtml. California Department of Fish and Game, Sacramento, CA.

CDFG. 2006b. State and federally listed endangered, threatened, and rare plants of California. California Naturally Diversity Database available at www.dfg.ca.gov/hcpb/species/t_e_spp/tespp.shtml. California Department of Fish and Game, Sacramento, CA.

Chin YP, Gschwend PM. 1992. Partitioning of poly cyclic aromatic hydrocarbons to marine pore-water organic colloids. *Environ Sci Technol* 26:1621-1626.

Crosby DG. 1998. *Environmental Toxicology and Chemistry*. Birks JW, editor. New York, NY: Oxford University Press.

CSIRO. 2001. BurrliOZ v. 1.0.13: Commonwealth Scientific and Industrial Research Organization, Australia.

CVRWQCB. 2004. The water quality control plan (basin plan) for the California Regional Water Quality Control Board Central Valley Region, fourth edition, the Sacramento and San Joaquin River basins. Central Valley Regional Water Quality Control Board, Rancho Cordova, CA.

Debruijn J, Busser F, Seinen W, Hermens J. 1989. Determination of octanol-water partition coefficients for hydrophobic organic chemicals with the slow-stirring method. *Environ Toxicol Chem* 8:499-512.

Dewolf W, Canton JH, Deneer JW, Wegman RCC, Hermens JLM. 1988. Quantitative structure activity relationships and mixture-toxicity studies of alcohols and chlorohydrocarbons - reproducibility of effects on growth and reproduction of *Daphnia magna*. *Aquat Toxicol* 12:39-49.

Dixon WJ. 1953. Processing Data for Outliers. *Biometrics* 9:74-89.

ECB. 2003. Technical guidance document on risk assessment in support of commission directive 93/67/EEC on risk assessment of new notified substances, commission regulation (EC) no. 1488/94 on risk assessment for existing substances, directive 98/8/EC of the European Parliament and of the Council concerning the placing of

biocidal products on the market. Part II. Environmental risk assessment. In: European Chemicals Bureau ECJRC, editor. European Communities.
ECOTOX. 2006. ECOTOX Code List, ECOTOXicology Database System, http://www.epa.gov/ecotox/help/codelist.htm. United States Environmental Protection Agency, Washington D. C.
Ellersieck, M.R., A. Asfaw, F.L. Mayer, G.F. Krause, K. Sun, and G. Lee. 2003. Acute-to-chronic estimation (ACE v. 2.0) with time-concentration-effect models: User manual and software. U.S. Environmental Protection Agency Report No. EPA/600/R-03/107, Washington, DC. 26 p. + software.
Felsot AS. 2005. A critical analysis of the draft report, "Amendments to the water quality control plan for the Sacramento River and San Joaquin River basins for the control of diazinon and chlorpyrifos runoff into the lower San Joaquin River," (Karkoski et al. 2004) and supporting documents. Prepared for the Central Valley Regional Water Quality Control Board, Sacramento, CA.
Finney DJ. 1942. The analysis of toxicity tests on mixtures of poisons. *Ann Appl Biol* 29:82-94.
Galassi S, Mingazzini M, Vigano L, Cesareo D, Tosato ML. 1988. Approaches to modeling toxic responses of aquatic organisms to aromatic hydrocarbons. *Ecotoxicol Environ Saf* 16:158-169.
Hermens J, Canton H, Janssen P, Dejong R. 1984. Quantitative structure activity relationships and toxicity studies of mixtures of chemicals with anesthetic potency - acute lethal and sublethal toxicity to *Daphnia magna*. *Aquat Toxicol* 5:143-154.
Host GE, Regal RR, Stephan CE. 1995. Analyses of acute and chronic data for aquatic life. United States Environmental Protection Agency, Washington, DC.
Konemann H. 1981. Quantitative structure-activity-relationships in fish toxicity studies. 1. Relationship for 50 industrial pollutants. *Toxicology* 19:209-221.
Kuhn R, Pattard M, Pernak KD, Winter A. 1989. Results of the harmful effects of water pollutants to *Daphnia magna* in the 21-day reproduction test. *Water Res* 23:501-510.
Mackay D. 1982. Correlation of bioconcentration factors. *Environ Sci Technol* 16:274-278.
Mackay D. 2001. *Multimedia Environmental Fate Models: The Fugacity Approach, Second Edition*. Boca Raton, FL: Lewis Publishers.
OECD. 1995. OECD environment monographs No. 92, OECD environmental health and safety publications, series on testing and assessment, No. 3, guidance document for aquatic effects assessment. Organization for Economic Co-operation and Development, Paris.
Plackett RL, Hewlett PS. 1952. Quantal responses to mixtures of poisons. *Journal of the Royal Statistical Society Series B-Statistical Methodology* 14:141-163.
RIVM. 2001. Guidance document on deriving environmental risk limits in The Netherlands. National Institute of Public Health and the Environment.
Sangster Research Laboratories. 2004. LOGKOW. A databank of evaluated octanol-water partition coefficients (Log P); http:// logkow.cisti.nrc.ca/logkow/index.jsp. Canadian National Committee for CODATA.
Siepmann S, Finlayson B. 2000. Water quality criteria for diazinon and chlorpyrifos. California Department of Fish and Game.

TenBrook PL, Tjeerdema RS. 2006. Methodology for derivation of pesticide water quality criteria for the protection of aquatic life in the Sacramento and San Joaquin River Basins. Phase I: Review of existing methodologies. Final Report. Central Valley Regional Water Quality Control Board, Rancho Cordova, CA.

TenBrook PL, Tjeerdema RS, Hann P, Karkoski J. 2009. Methods for deriving pesticide aquatic life criteria. *Reviews of Environmental Contamination and Toxicology*.199:19-109.

USEPA. 1980a. Ambient water quality criteria for aldrin/dieldrin. United States Environmental Protection Agency, Washington D. C.

USEPA. 1980b. Ambient water quality criteria for chlordane, EPA 440/5-80-027. United States Environmental Protection Agency, Washington D. C.

USEPA. 1980c. Ambient water quality criteria for endosulfan, EPA 440/5-80-046. United States Environmental Protection Agency, Washington D. C.

USEPA. 1980d. Ambient water quality criteria for endrin, EPA 440/5-80-047. United States Environmental Protection Agency, Washington D. C.

USEPA. 1985. Guidelines for deriving numerical national water quality criteria for the protection of aquatic organisms and their uses, PB-85-227049. United States Environmental Protection Agency, National Technical Information Service, Springfield, VA.

USEPA. 1996a. Product properties test guidelines. OPPTS 830.7560. Partition coefficient (n-octanol/water), generator column method, EPA 712-C-96-039. United States Environmental Protection Agency, Washington D. C.

USEPA. 1996b. Product properties test guidelines. OPPTS 830.7550. Partition coefficient (n-octanol/water), shake flask method, 712-C-96-038. United States Environmental Protection Agency, Washington D. C.

USEPA. 2002. Short-term methods for estimating the chronic toxicity of effluents and receiving waters to freshwater organisms, 4th edition, EPA-821-R-02-013. United States Environmental Protection Agency, Washington, D. C.

USEPA. 2003a. 2003 Draft update of ambient water quality criteria for copper, EPA 822-R-03-026. United States Environmental Protection Agency, Washington D. C.

USEPA. 2003b. Water quality guidance for the Great Lakes system. *Federal Register* 40.

USEPA. 2005. Aquatic life ambient water quality criteria, diazinon, final, EPA-822-R-05-006. United States Environmental Protection Agency, Washington D. C.

USEPA. 2006. Recognition and management of pesticide poisonings, 5th edition, Section IV, Chapter 16 Fumigants. United States Environmental Protection Agency, Washington D. C.

Van Den Berg M, Birnbaum L, Bosveld ATC, Brunstrom B, Cook P, Feeley M, Giesy JP, Hanberg A, Hasegawa R, Kennedy SW, Kubiak T, Larsen JC, Van Leeuwen FXR, Liem AKD, Nolt C, Peterson RE, Poellinger L, Safe S, Schrenk D, Tillitt D, Tysklind M, Younes M, Waern F, Zacharewski T. 1998. Toxic equivalency factors (TEFs) for PCBs, PCDDs, PCDFs for humans and wildlife. *Environ Health Perspect* 106:775-792.

Van Der Hoeven N, Noppert F, Leopold A. 1997. How to measure no effect .1. Towards a new measure of chronic toxicity in ecotoxicology, introduction and workshop results. *Environmetrics* 8:241-248.

Van Leeuwen CJ, Adema DMM, Hermens J. 1990. Quantitative structure-activity-relationships for fish early life stage toxicity. *Aquat Toxicol* 16:321-334.

Van Leeuwen CJ, Vanderzandt PTJ, Aldenberg T, Verhaar HJM, Hermens JLM. 1992. Application of QSARs, extrapolation and equilibrium partitioning in aquatic effects assessment. 1. Narcotic industrial pollutants. *Environ Toxicol Chem* 11:267-282.

Varó I, Serrano R, Pitarch E, Amat F, Lopez FJ, Navarro JC. 2002. Bioaccumulation of chlorpyrifos through an experimental food chain: Study of protein HSP70 as biomarker of sublethal stress in fish. *Arch Environ Contam Toxicol* 42:229-235.

Veith GD, Call DJ, Brooke LT. 1983. Structure toxicity relationships for the fathead minnow, *Pimephales promelas* - narcotic industrial chemicals. *Can J Fish Aquat Sci* 40:743-748.

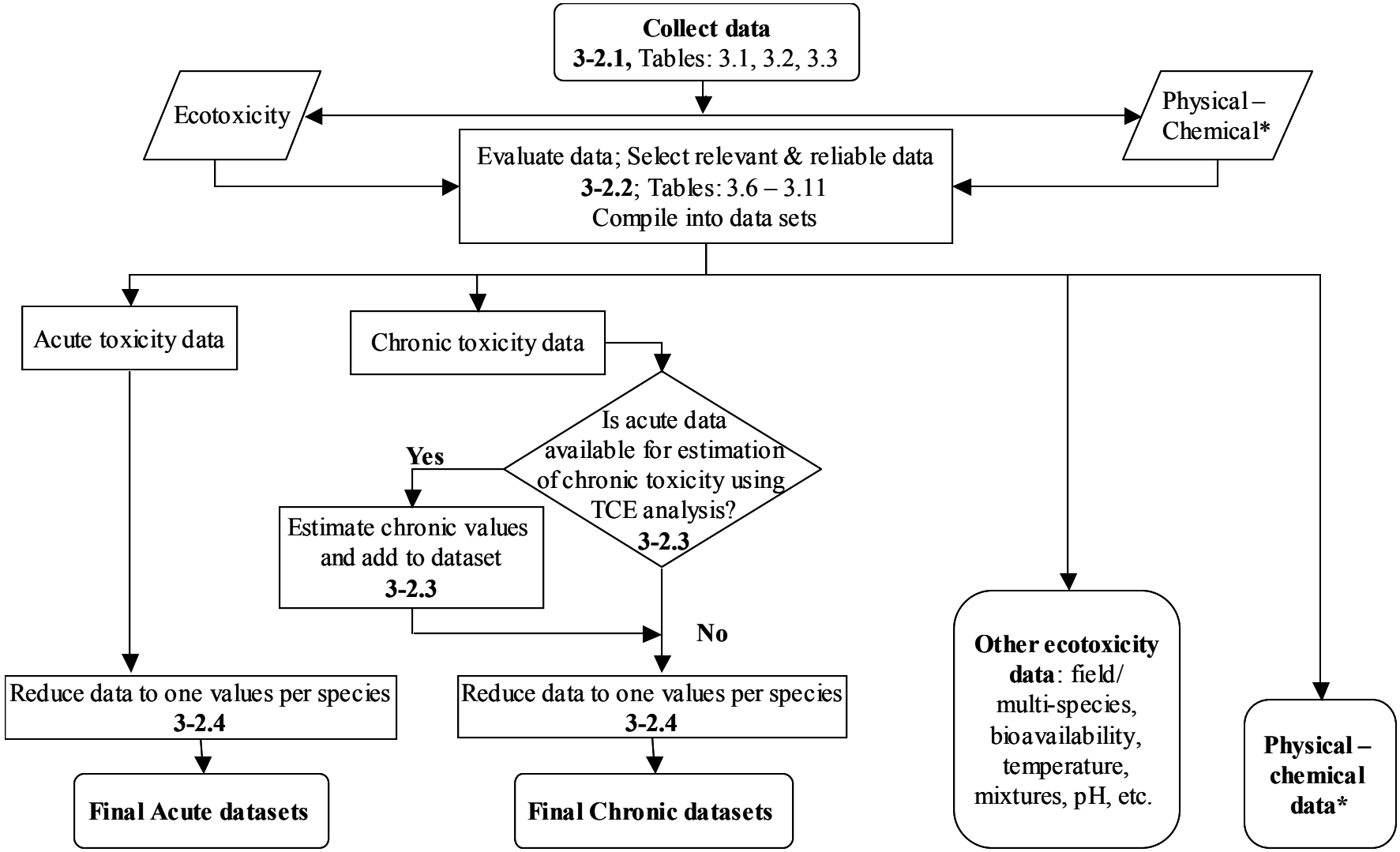
Verhaar HJM, Van Leeuwen CJ, Bol J, Hermens JLM. 1994. Application of QSARs in risk management of existing chemicals. *SAR QSAR Environ Res* 2:39-58.

Zabel TF, Cole S. 1999. The derivation of environmental quality standards for the protection of aquatic life in the UK. *Journal of the Chartered Institution of Water and Environmental Management* 13:436-440.

Figures and Tables

Figure 3.1 Data flow

For more information on each process in the chart, see the listed tables and section references (listed in bold).



See Fig 3.2 for use of data sets

* Physical-chemical data is used for ecotoxicity data evaluation and in some of the considerations after criteria are derived

Figure 3.2 Criteria derivation flow chart

To begin, see Sections 3-3.0, 3-4.0, and Figure 3.1. For more information on each process in the chart, see the listed tables and section references (listed in bold). If plants/algae are most sensitive, refer to section 3-4.3 instead

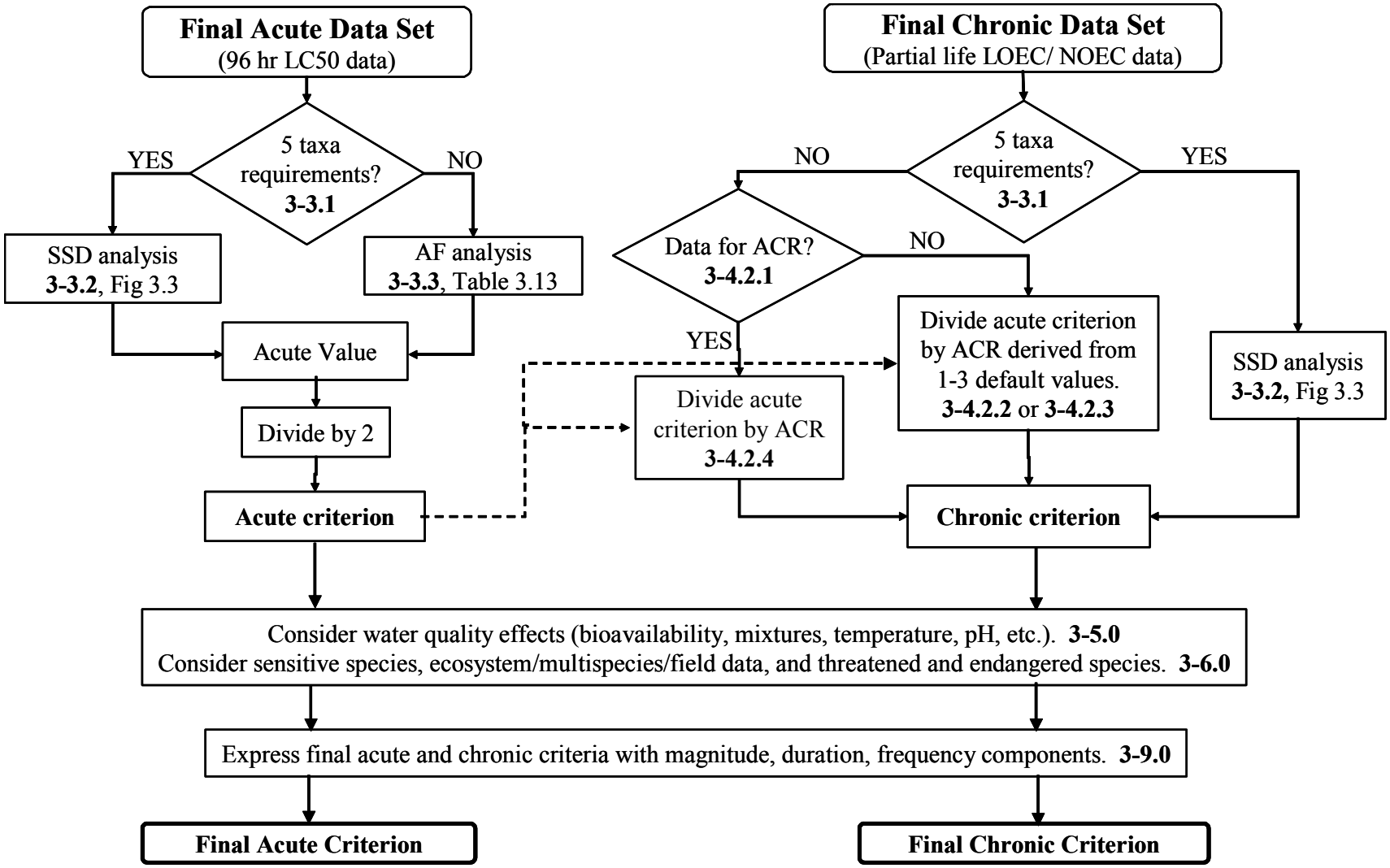
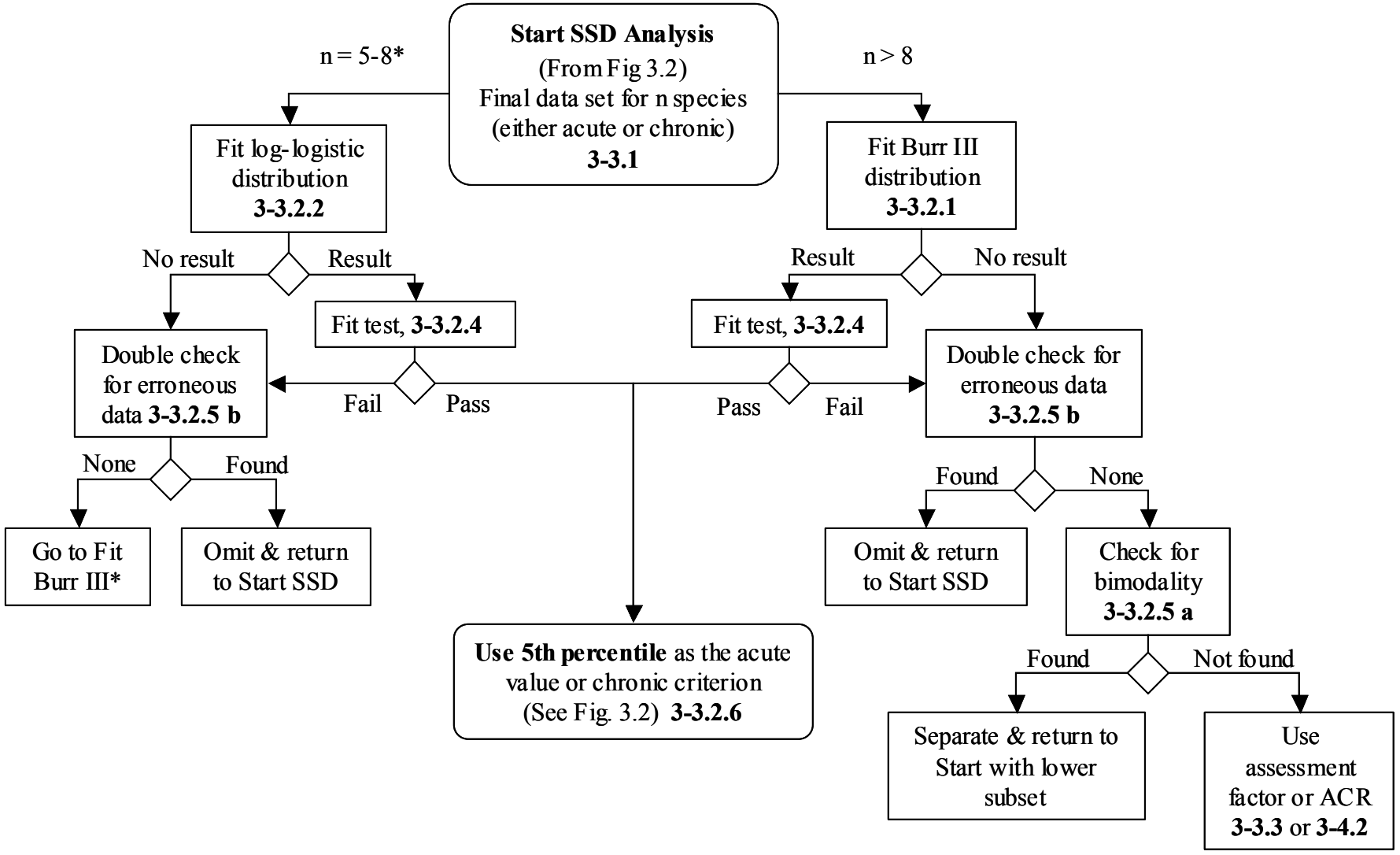


Figure 3.3 SSD flow chart

The 5 taxa requirements should be met before using a distribution, (exception for subset of a multi-modal data set, section **3-3.2.5 a)**. For more information on each process in the chart, see the listed tables and section references (listed in bold).



* When n (taxa requirements) = 5-8, the log-logistic distribution is preferred, but Burr III may be used if it cannot be fit

Figure 3.4 Data summary sheet (2 pages)

Toxicity Data Summary

Study:

Relevance
Score:
Rating:

Reliability
Score:
Rating:

Reference		
Parameter	**Value**	**Comment**
Test method cited		
Phylum		
Class		
Order		
Family		
Genus		
Species		
Family in North America?		
Age/size at start of test/growth phase		
Source of organisms		
Have organisms been exposed to contaminants?		
Animals acclimated and disease-free?		
Animals randomized?		
Test vessels randomized?		
Test duration		
Data for multiple times?		
Effect 1		
Control response 1		
Effect 2		
Control response 2		
Effect 3		
Control response 3		
Temperature		
Test type		
Photoperiod/light intensity		
Dilution water		
pH		
Hardness		
Alkalinity		

Reference		
Parameter	**Value**	**Comment**
Conductivity		
Dissolved Oxygen		
Feeding		
Purity of test substance		
Concentrations measured?		
Measured is what % of nominal?		
Chemical method documented?		
Concentration of carrier (if any) in test solutions		
Concentration 1 Nom/Meas (µg/L)		Reps and # per (cell density for single-celled organisms):
Concentration 2 Nom/Meas (µg/L)		Reps and # per (cell density for single
Concentration 3 Nom/Meas (µg/L)		Reps and # per (cell density for single
Concentration 4 Nom/Meas (µg/L)		Reps and # per (cell density for single
Concentration 5 Nom/Meas (µg/L)		Reps and # per (cell density for single
Control		Reps and # per (cell density for single
LCx; indicate calculation method		
ECx; indicate calculation method		
NOEC; indicate calculation method, significance level (p-value) and minimum significant difference (MSD)		Method: p: MSD:
LOEC; indicate calculation method		
MATC (GeoMean NOEC,LOEC)		
% control at NOEC		
% of control LOEC		

Other notes:

Table 3.1 Data sources. Original sources identified through handbooks, review articles, etc., should be evaluated.

Source	Details/Notes	Date(s)
U.S. Environmental Protection Agency EPA re-registration eligibility decision (RED) or interim re-registration eligibility decision (IRED)	Review RED or IRED on compound and EPA Office of Pesticide Programs database (ipmcenters.org/Ecotox/). Submit Freedom of Information Act (FOIA) request for relevant studies by completing an Affirmation of Non-Multinational Status form, available here: epa.gov/pesticides/foia/affirmation.htm, and sending with list of the study MRID numbers and info about yourself and who you work for, to: hq.foia@epa.gov	
California Department of Pesticide Regulation	Find relevant study numbers in the pesticide database: http://apps.cdpr.ca.gov/ereglib/ To retrieve studies, contact Registration Branch of DRP: Jacquelyn Rivers: Jrivers@cdpr.ca.gov, or Rachel Kubiak: (916) 324-3939, rkubiak@cdpr.ca.gov.	
California Department of Fish and Game- Aquatic Toxicity Laboratory	Contact or check online for lab reports or criteria reports, may be available through DPR	
University Libraries		
Electronic databases	See Table 3.2 for list and details	
Handbooks		
ECETOC	Aquatic toxicity data evaluation.	1993
Howard	Handbook of environmental fate and exposure data for organic chemicals. Vol. III: Pesticides	1991
Mackay et al.	Illustrated handbook of physical-chemical properties and environmental fate for organic chemical. Volume V. Pesticide chemicals	Book: 1997 CD-ROM: 1999
MITI	Biodegradation and bioaccumulation data on existing data based on the CSCL Japan	1992
Nikunen et al.	Environmental properties of chemicals	2003
Verschueren	Handbook of environmental data on organic chemicals, 2nd edition	Print: 1983 CD-ROM: 2001
Others		

Table 3.1 Data sources. Original sources identified through handbooks, review articles, etc., should be evaluated.

Source	Details/Notes	Date(s)
Review articles		
e.g., Racke	Environmental fate of chlorpyrifos	1993
e.g., Laskowski	Physical and chemical properties of pyrethroids	2002
Internal databases		
International criteria documents/government reports	Often available via the Internet	
Laboratory reports		
Manufacturer data	May be listed in RED/ IRED, EPA OPP database and available from EPA, may be proprietary,	
Memos	May be listed in RED/ IRED, EPA OPP database and available from EPA	
Registration packets	Studies used for pesticide registration may be listed in RED/ IRED, EPA OPP database and available from EPA, packets can be difficult to obtain	

Table 3.2 Web addresses for various electronic resources.

Database	Description/contents	URL
CLOGP	K_{ow} calculator available through Bio-Loom	www.biobtye.com
BIOSIS	Bibliographic; multidisciplinary	http://www.biosis.org/
ChemFinder	Physical Properties; chemical structures, names and physical properties	http://www.chemfinder.com
Chemical Abstracts	Bibliographic; primarily chemistry, life sciences	http://www.cas.org/
Current Contents	Bibliographic: multidisciplinary	http://scientific.thomson.com/products/ccc/
ECOTOX (was AQUIRE)	Single chemical toxicity information for aquatic and terrestrial life	http://www.epa.gov/ecotox/
EFDB	Environmental Fate Data Base; access to DATALOG, BIOLOG, CHEMFATE, BIODEG	http://www.syrres.com/esc/efdb.htm
DATALOG	Bibliographic; environmental fate	
BIOLOG	Microbial toxicity and biodegradation	
CHEMFATE	Environmental fate and chemical-physical properties	
BIODEG	Biodegradation data	
EXTOXNET	Extension Toxicology Network; pesticide profiles and toxicology information	http://extoxnet.orst.edu/
Estimation Program Interface Suite	Tools from USEPA for estimation of numerous physical-chemical parameters	http://www.epa.gov/oppt;exposure/docs/episuite.htm
KowWin	Octanol-water partition coefficient program. Syracuse Research Corporation, New York, NY.	http://www.syrres.com/esc/est_soft.htm
LOGKOW	Sangster Research Laboratories	http://logkow.cisti.nrc.ca/logkow/index.jsp
Pesticide Action Network	Bibliographic; toxicity and regulatory information for pesticides	http://www.pesticideinfo.org/Index.html
PHYSPROP	Physical Properties; chemical structures, names and physical properties	http://www.syrres.com/esc/physprop.htm

Table 3.2 Web addresses for various electronic resources.

Database	Description/contents	URL
Pesticide Ecotoxicity Database	USEPA Office of Pesticide Programs toxicity database for registered pesticides, mostly unpublished studies, see EPA entry in Table 3.1	http://www.ipmcenters.org/Ecotox
POLTOX via OVID	Bibliographic; pollution and toxicology; plants, animals, and humans.	http://www.ovid.com
PubMed	Bibliographic; medicine, life sciences, molecular biology, genetics, others	http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?DB=pubmed
TOXNET	Access to HSDB, TOXLINE, IRIS	http://toxnet.nlm.nih.gov/
HSDB	Hazardous Substances Data Bank	
TOXLINE	Toxicology Literature Online	
IRIS	Integrated Risk Information System	
TSCATS	Bibliographic; Toxic Substances Control Act submission data	http://www.syrres.com/esc/tscats.htm
Web of Science	Bibliographic; access to Institute for Scientific Information Citation Databases	http://scientific.thomson.com/products/wos/

Table 3.3 Kinds of data that should be collected for criteria derivation.

Category	Data
Physical-chemical	BAF (bioaccumulation factor)
	BCF (bioconcentration factor)
	BMF (biomagnification factor)
	CAS (chemical abstract service number)
	Chemical formula
	Density
	IUPAC name
	K_H (Henry's Law constant)
	Log K_d (solid-water partition coefficient)
	Log K_{DOC} (dissolved organic carbon-water partition coefficient)
	Log K_{OC} (organic carbon-water partition coefficient)
	Log K_{ow} (octanol-water partition coefficient)
	Melting point
	Molecular weight
	pK_a (acid dissociation constant)
	S (aqueous solubility)
	Structure
	$t_{1/2}$ (half-life), hydrolysis, photolysis, biotic degradation
	Vapor pressure
Ecotoxicity	Acute (survival, immobilization)
	Aquatic insects
	Aquatic plants
	Bioavailability
	Chemical mixtures
	Chronic (survival, growth, reproduction, embryonic/shell development, hatching, germination, behavior effects, enzyme inhibition, endocrine disruption, other physiological effects, insect control, changes in species diversity or abundance)
	Field
	Fish
	Insects
	Laboratory
	Mesocosm
	Microcosm
	Multi-species
	Non-insect aquatic invertebrates
	Single chemical
	Single-species
	Wildlife
Human health	FDA action levels

Table 3.4 Acceptable methods for determination of physical-chemical parameters, other than the octanol-water partition coefficient, K_{ow}.

Constant	Method	Notes	Reference
Bioconcentration Factor, BCF	Flow-through; fish	Determines apparent steady state BCF	OECD 305 (1996)
	Flow-through; fish and mollusks	Determines apparent steady state BCF	ASTM E 1022-94 (2002a)
Dissociation, pK_a	Conductometric	Onsager (1927) equation must hold; Acid/base dissociations; Non-acid/base dissociations	OECD 112 (1981)
	Spectrophotometric	Solubility: low to high; Differential uv/vis absorption for ionized vs. unionized species; Acid/base dissociations; Non-acid/base dissociations	"
	Titration	Solubility: moderate to high	"
Hydrolysis Rate	Tiered approach	Determines rate in acidic, basic and neutral conditions	ASTM E895-89 (2001a)
	Tiered approach	Determines rate in acidic, basic and neutral conditions	OECD 111 (2004)
Solid-water partition,	Batch Equilibrium	Colloidal binding can reduce accuracy	ASTM E 1195-01 (2001b)
K_d, K_{oc}	Batch Equilibrium	Colloidal binding can reduce accuracy	OECD 106 (2000)
	Batch Equilibrium Co-solvent	Corrects for colloid binding	Evers & Smedes (1993)
	HPLC	Estimation technique	OECD 121 (2001)
Solubility, S	Column Elution	Solubility $< 10^{-2}$ g/L	OECD 105 (1995b)
	Flask	Solubility $> 10^{-2}$ g/L	"
	Flask	Solubility $\geq$ 1 mg/L	ASTM E 1148-02 (2002b)
	Generator Column	Solubility < 1 mg/L	"
	Nephelometric	Solubility $\geq$ 1 mg/L	"

Table 3.5 Acceptable experimental and computational techniques for determination of the octanol-water partition coefficient, K_{ow}, and the priority for their use (USEPA 2003a).

Log K_{ow} < 4

Method	Reference	Priority
Slow stir	Debruijn *et al.* (1989)	1
Generator-column	USEPA (1996a)	1
Shake-flask	USEPA (1996b)	1
HPLC w/ extrapolation to 0% solvent	ASTM E 1147-92 (1997)	2
HPLC w/o extrapolation to 0% solvent	ASTM E 1147-92 (1997)	3
CLOGP program	Through Bio-Loom at www.biobtye.com	4

Log K_{ow} > 4

Method	Reference	Priority
Slow stir	Debruijn *et al*. (1989)	1
Generator-column	USEPA (1996a)	1
HPLC w/ extrapolation to 0% solvent	ASTM E 1147-92 (1997)	2
HPLC w/o extrapolation to 0% solvent	ASTM E 1147-92 (1997)	3
Shake-flask	USEPA (1996b)	4
CLOGP program	Through Bio-Loom at www.biobtye.com	5

Table 3.6 Rating of relevance/usability of data for derivation of criteria.

Parameter	Score
Acceptable standard (or equivalent) method used	10
Endpoint linked to survival/growth/reproduction	15
Freshwater	15
Chemical $\geq$ 80% pure	15
Species is in a family that resides in North America	15
Toxicity value calculated or calculable (e.g., LC_{50})	15
Controls	15
Described (i.e., solvent, dilution water, etc.)	7.5
Response reported and meets acceptability requirements	7.5
Total	100

Table 3.7 Documentation rating for aquatic laboratory data (adapted from ECOTOX 2006). Full score is given if parameter is reported; 0 score is given if not.

Parameter[1]	**Score**[2]
Results published or in signed, dated format	6
Exposure duration	12
Control type	8
Organism information (i.e., age, life stage, etc.)	
Source	5
Age/life stage/size/growth phase	5
Chemical	
Grade or purity	5
Analytical method (if measured)	4
Nominal concentrations	3
Measured concentrations	3
Exposure type	5
Dilution water source	3
Hardness	2
Alkalinity	2
Dissolved oxygen	4
Temperature	4
Conductivity	2
pH	3
Photoperiod and/or light intensity (plant studies must include intensity)	3
Statistics	
Methods identified	5
Hypothesis tests	
Statistical significance	2
Significance level	2
Minimum significant difference	2
% of control at NOEC and/or LOEC	2
Point estimates (i.e. LC50, EC25, etc.)	8
Total	100

[1] Compiled from RIVM (2001), USEPA (1985; 2003b), ECOTOX (2006), CCME (1999), ANZECC & ARMCANZ (2000), OECD (1995), and Van Der Hoeven *et al*. (1997).

[2] Weighting based acceptability criteria from various ASTM, OECD, APHA, and USEPA methods, ECOTOX (2006), and on data quality criteria in RIVM (2001), USEPA (1985; 2003b), CCME (1999), ANZECC & ARMCANZ (2000), OECD (1995), and Van Der Hoeven *et al*. (1997).

Table 3.8 Acceptability rating for aquatic laboratory data (adapted from ECOTOX 2006). Score is given if parameter met standard test guidance; score of 0 is given if parameter was not reported or did not meet test guidance.

Parameter	Score
Acceptable standard (or equivalent) method used (e.g., ASTM, USEPA, OECD, APHA)	5
Test was of appropriate duration	2
Control	
Appropriate (e.g., solvent control included, if carrier was used)	6
Response within test guidance	9
Chemical	
Purity > 80% pure	10
Measured concentrations within 20% of nominal	4
Concentrations do not exceed 2x water solubility	4
Carrier solvent $\leq$ 0.5 mL/L (acute); $\leq$ 0.1 mL/L (chronic); score 4 if not used	4
Organisms	
Appropriate size/age/growth phase	3
No prior contaminant exposure	4
Organisms randomly assigned to test containers	1
Adequate number per replicate/appropriate cell density	2
Organisms fed 2 h before solution renewal or not fed in acute tests; fed appropriately in chronic tests	3
Organisms properly acclimated and disease-free prior to testing	1
Exposure type and renewal frequency appropriate to chemical	2
Dilution water source acceptable	2
Hardness within organism tolerance and/or dilution water specifications	2
Alkalinity within organism tolerance and/or dilution water specifications	2
Dissolved oxygen $\geq$ 60%	6
Temperature within organism tolerance (3 pts) and/or test guidance and held to $\pm$ 1^{o}C (3 pts)	6
Conductivity within organism tolerance and/or dilution water specifications	1
pH within organism tolerance and/or dilution water specifications	2
Photoperiod and light intensity within organism tolerance and/or test guidance	2
Statistics	
Adequate number of concentrations	3
Random or random block design employed	2
Adequate replication	2
Appropriate spacing between concentrations (dilution factor $\geq$ 0.3)	2
Appropriate statistical method used	2
Hypothesis tests	
Minimum significant difference (MSD) below recommended upper bound[3]	1
NOEC response reasonable compared to control[4]	1
LOEC response reasonable compared to control[4]	1
Point estimates	
LC/EC values calculable (i.e., no < or > results)	3
Total	100

[1] Compiled from RIVM (2001), USEPA (1985; 2003b), ECOTOX (2006), CCME (1999), ANZECC & ARMCANZ (2000), OECD (OECD 1995), and Van Der Hoeven *et al*. (1997).
[2] Weighting based acceptability criteria from various ASTM, OECD, APHA, and USEPA methods, ECOTOX (2006), and on data quality criteria in RIVM (2001), USEPA (1985; 2003b), CCME (1999), ANZECC & ARMCANZ (2000), OECD (1995), and Van Der Hoeven *et al*. (1997).
[3] Acceptable MSD levels are species and test-method specific; see USEPA (2002) for upper bounds for several standard test species.
[4] Reasonableness is decided using professional judgment on a case-by-case basis, based on MSD upper bound and potential biological significance of response level.

Table 3.9 Documentation and acceptability rating for aquatic outdoor field data and indoor model ecosystems (adapted from ECOTOX 2006).

Parameter[1]	Score[2]
Results published or in signed, dated format	5
Exposure duration and sample regime adequately described	6
Unimpacted site (score 7 for artificial systems)	7
Adequate range of organisms in system (1^o producers, 1^o, 2^o consumers)	6
Chemical	
Grade or purity stated	6
Concentrations measured and reported	2
Analysis method stated	2
Habitat described (e.g., pond, lake, ditch, artificial, lentic, lotic, etc.)	6
Water Quality	
Source identified	3
Hardness reported	2
Alkalinity reported	2
Dissolved oxygen reported	2
Temperature reported	2
Conductivity reported	2
pH reported	2
Photoperiod reported	2
Organic carbon reported	2
Chemical fate reported	3
Geographic location identified (score 2 for indoor systems)	2
Pesticide application	
Type reported (e.g., spray, dilutor, injection, etc.)	2
Frequency reported	2
Date/season reported (score 2 for indoor systems)	2
Test endpoints	
Species abundance reported	3
Species diversity reported	3
Biomass reported	2
Ecosystem recovery reported	2
Statistics	
Methods identified	2
At least 2 replicates	3
At least 2 test concentrations and 1 control	3
Dose response observed	2
Hypothesis tests	
NOEC determined	4
Significance level stated	2
Minimum significant difference reported	2
% of control at NOEC and/or LOEC reported or calculable	2
Total	100

[1] Compiled from RIVM (2001), USEPA (1985; 2003b), ECOTOX (2006), CCME (1999), ANZECC & ARMCANZ (2000), OECD (1995), and Van Der Hoeven *et al*. (1997).
[2] Weighting based ECOTOX (2006) and on data quality criteria in RIVM (2001) and OECD (1995).

Table 3.10 Documentation and acceptability rating for terrestrial laboratory/field data (adapted from ECOTOX 2006). Score is given if parameter is reported.

Parameter[1]	**Score**[2]
Exposure duration	20
Control type	7
Organism information (i.e. age, life stage, etc.)	8
Chemical grade or purity	5
Chemical analysis method	5
Exposure type (i.e., dermal, dietary, gavage, etc.)	10
Test location (i.e., laboratory, field, natural artificial)	5
Application frequency	5
Organism source	5
Organism number and/or sample number	5
Dose number	5
Statistics	
Hypothesis tests	
Statistical significance	5
Significance level	5
Minimum significant difference	3
% of control at NOEC and/or LOEC	3
Point estimates (i.e. LC50, EC25, etc.)	4
Total	100

[1] Compiled from ECOTOX (2006) and Van Der Hoeven *et al*. (1997).
[2] Weighting based on ECOTOX (2006).

Table 3.11 Data categories based on relevance and reliability scores. N = not relevant/not reliable; L = less relevant/reliable; R = relevant, reliable. Unshaded category is used for criteria derivation; light shaded category is used for supporting data; dark shaded category is not usable.

	Reliability			
	Score	0-59	60-73	74-100
Relevance	0-69	NN	LN	RN
	70-89	NL	LL	RL
	90-100	NR	LR	RR

Table 3.12 Extrapolation constants, k, for median and lower 95% confidence limit estimates of the 5th percentile value using a log-logistic distribution (taken from Aldenberg & Slob 1993).

n	Median	Lower 95% confidence limit
2	2.49	27.7
3	2.05	8.14
4	1.92	5.49
5	1.85	4.47
6	1.81	3.93
7	1.78	3.59
8	1.76	3.37
9	1.75	3.19
10	1.73	3.06
11	1.72	2.96
12	1.72	2.87
13	1.71	2.80
14	1.70	2.74
15	1.70	2.68
20	1.68	2.49
30	1.66	2.28
50	1.65	2.10
100	1.64	1.95
200	1.63	1.85
500	1.63	1.76
∞	1.62	1.62

Table 3.13 Assessment factors to apply to lowest acute toxicity values in data sets that meet fewer than 5 of the taxa requirements.

Number of taxa requirements	Factor
1	57 x 10[1]
2	36
3	7.8
4	5.1
5[2]	3.8

[1] The factor 57 was derived from pesticide data; the 10 is an additional factor assessed to protect against cases in which Daphnids are among the most tolerant species.

[2] This factor is provided for use if the data requirements are met, but the SSD cannot be fit.

Table 3.14 Calculation of default acute-to-chronic ratio (ACR)

Chemical	**ACR**
Chlordane	14[1]
Chlorpyrifos	2.2[2]
Diazinon	3.0[3]
Dieldrin	8.5[1]
Endosulfan	3.9[1]
Endrin	4.0[1]
Lindane	25[1]
Parathion	10[1]
80th percentile	12.4

[1] Host *et al*. (1995)
[2] This methodology
[3] Siepmann & Finlayson (2000)

Table 3.15 Default BMF values (ECB 2003)

Log K_{ow}	BCF	BMF
< 4.5	< 2,000	1
4.5 - < 5	2,000-5,000	2
5 – 8	5,000	10
> 8 – 9	2,000-5,000	3
> 9	< 2,000	1

Table 3.16. QSARS for estimating toxicity from K_{ow} for chemicals acting by narcosis; from OECD (1995) and RIVM (2001).

Species	Equation
Acute Toxicity	Summarized in OECD 1995a
Pimephales promelas	log LC_{50} (mM) = -0.94 log K_{ow} + 0.94 log (0.00068 K_{ow} + 1) + 1.75 (Veith *et al.* 1983)
Poecilia reticulata	log LC_{50} (mM) = -0.87 log K_{ow} + 1.87 (Konemann 1981)
Daphnia magna	log EC_{50} (mM) = -0.91 log K_{ow} + 1.72 (Hermens *et al.* 1984)
Chronic Toxicity	Summarized in OECD (1995)
Brachydanio rerio/ *Pimephales promelas*	log NOEC (mM) = -0.90 log K_{ow} + 0.8 (Call *et al.* 1985; Van Leeuwen *et al.* 1990)
Daphnia magna	log NOEC (mM) = -1.04 log K_{ow} + 1.30 (Dewolf *et al.* 1988; Kuhn *et al.* 1989)
Daphnia magna	log NOEC (mM) = -1.07 log K_{ow} + 1.25 (Dewolf *et al.* 1988)
Selenastrum capricornutum	log NOEC (mM) = -1.00 log K_{ow} + 1.77 (Calamari *et al.* 1983; Galassi *et al.* 1988)
Chronic Toxicity	Summarized in RIVM (2001) from Van Leeuwen *et al*. (1992); Verhaar *et al*. (1994)
Skeletonema costacum	log NOEC (M) = -0.72 log K_{ow} - 1.42
Scenedesmus subspicatus	log NOEC (M) = -0.86 log K_{ow} – 1.41
Selenastrum capricornutum	log NOEC (M) = -1.00 log K_{ow} - 1.71
Tetrahymena pyriformis	log NOEC (M) = -0.80 log K_{ow} - .128
Lymnaea stagnalis	log NOEC (M) = -0.86 log K_{ow} – 2.08
Nitocra spinipes	log NOEC (M) = -0.78 log K_{ow} – 2.14
Daphnia magna	log NOEC (M) = -1.04 log K_{ow} – 1.70
Aedes aegypti	log NOEC (M) = -1.09 log K_{ow} – 1.36
Culex pipiens	log NOEC (M) = -0.86 log K_{ow} – 1.98
Brachydanio rerio/ Pimephales promelas	log NOEC (M) = -0.87 log K_{ow} – 2.35
Ambystoma mexicanum	log NOEC (M) = -0.88 log K_{ow} – 1.89
Rana temporaria	log NOEC (M) = - 1.09 log K_{ow} – 1.47
Xenopus laevis	log NOEC (M) = -0.90 log K_{ow} – 1.79